Dynamics of and on Complex Networks

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Abstract

Complex networks are dynamic, evolving structures that can host a great number of dynamical processes. In this thesis, we address current challenges regarding the dynamics of and dynamical processes on complex networks. First, we study complex network dynamics from the standpoint of network growth. As a quantitative measure of the complexity and information content of networks generated by growing network models, we define and evaluate their entropy rate. We propose stochastic growth models inspired by the duplication-divergence mechanism to generate epistatic interaction networks and find that they exhibit the property of monochromaticity as a result of their dynamical evolution. Second, we explore the dynamics of quantum mechanical processes on complex networks. We investigate the Bose-Hubbard model on annealed and quenched scale-free networks as well as Apollonian networks and show that their phase diagram changes significantly in the presence of complex topologies, depending on the second degree of the degree distribution and the maximal eigenvalue of the adjacency matrix. We then study the Jaynes-Cummings-Hubbard model on various complex topologies and demonstrate the importance of the maximal eigenvalue of the hopping matrix in determining the phase diagram of the model. Third, we investigate dynamical processes on interacting and multiplex networks. We study opinion dynamics in a simulated setting of two antagonistically interacting networks and recover the importance of connectivity and committed agents. We propose a multiplex centrality measure that takes into account the connectivity patterns within and across different layers and find that the dynamics of biased random walks on multiplex networks gives rise to a centrality ranking that is different from univariate centrality measures. Finally, we study the statistical mechanics of multilayered spatial networks and demonstrate the emergence of significant link overlap and improved navigability in multiplex and interacting spatial networks.
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Chapter 1

Introduction

In the past fifteen years, network science has undoubtedly emerged as a prominent inter-disciplinary field, benefiting from the expertise of many diverse fields, yet self-contained enough to have a language and set of tools of its own. As large scale empirical data on biological, technological and social systems became more and more widespread, the power of representing these real-world systems as complex networks has increasingly been recognized. As a result, this period has seen great advances in the theoretical framework of complex networks as well as the development of models and computational tools to describe and analyze the structure and dynamics of networks [1–3]. Many unifying principles underlying the structure of these diverse types of real-world networks, such as strong inhomogeneity, high clustering and compactness (small average path length), have been successfully characterized.

Perhaps even more important than characterizing the architecture of complex networks is identifying the collective behavior and dynamics of the interacting elements of these networks. Almost all real-world networks are not static but evolving, temporally or spatially or both, making them inherently dynamic [4]. Moreover, complex networks, be it equilibrium (static) or non-equilibrium (growing), can sustain many types of dynamical processes such as epidemic spreading and diffusion; synchronization; information spreading and opinion formation; traffic and congestion; random walks, search and navigation; percolation, condensation and other phase transitions [5, 6]. With their strong disorder, meaning huge fluctuations of vertex characteristics such as degrees with respect to the mean, complex networks provide a whole new substrate for these dynamical processes. In fact, it has been shown that many types of critical phenomena have significantly different
properties on complex topologies. Growing network models proposed to reproduce the heterogeneous architectures of real-world networks have been shown to undergo structural phase transitions. Adding one more layer of complexity to the subject, it is now becoming clear that the characteristics of dynamical processes are changed yet again when they take place on multiple layers of interacting complex networks instead of single networks [7].

Their evolving nature, the novel critical phenomena induced by the their structural properties, and the sheer abundance of dynamical processes that can be studied on them makes complex networks a very fertile field for statistical physicists. In fact, it is fair to say that the statistical physics community has been the biggest contributor to the field of complex networks, owing to these connections. After all, focusing on the cooperative dynamics and macroscopic properties of a system rather than the details of its constituents is not unfamiliar to statistical physicists.

In this dissertation, I present my contributions to the field of complex networks [8–14] where I use the methods of statistical physics and information theory to study social, biological, transportation and quantum networks, which are systems that are ostensibly distinct, yet unified by the common theme of dynamics. In particular, I address the subject of “dynamics of and on networks” from the perspectives of the dynamics of network growth, dynamics of quantum critical processes, dynamical processes on interacting and multiplex networks and finally, the statistical mechanics of multiplex and interacting spatial networks.

As part of the original work of this thesis, we will first investigate unexplored aspects of network growth. As a step towards developing an information theory of complex networks, we will propose a complexity measure, namely the entropy rate, as a way to quantify the complexity of growing network models. We will see that stochastic models of network growth can be devised as a possible means to explain the emergence of a modularity feature in genetic interaction networks. We will take a brief intermission from real-world networks to concentrate on the theory of quantum dynamical processes on complex topologies and see that beyond classical phase transitions, the dynamics of systems defined by quantum mechanical models and the quantum phase transitions within these models are also affected profoundly by the presence of complex topologies. We will then venture into the emerging subfield of interacting and multiplex networks and demonstrate some novel examples of dynamical processes on these networks. We shall see that, for instance, we
can model an election campaign as a dynamic opinion formation process between two antagonistically interacting networks and recover with a simple mathematical model the importance of connectivity and committed agents. We will see that by proposing a new multiplex centrality measure, we witness that the dynamics of biased random walks and centrality changes the outcome of a ranking process when the interactions between different layers of a multiplex is taken into account. We will finally see how overlap naturally emerges when the multiplex networks are also spatial and what the implications on navigability are when interacting transportation networks are considered.

The subject flow of the dissertation is outlined below:

In the rest of this chapter, we review the basics of network theory. Starting with a historical account of the milestones that were instrumental in the conception of network science, we proceed to summarize the terminology related to networks and then finally describe the fundamental network characteristics and the most important network models.

Chapter 2 of the dissertation tackles the question of dynamical evolution of complex networks from the standpoint of network growth. Models proposed as growth mechanisms that reproduce the defining structural characteristics of real-world networks have been a significant theme in network science since its earliest days. The purpose of this chapter in relation to growing networks is twofold: First, we address the problem of quantifying the complexity and information content of growing network models by introducing the entropy rate and calculating it analytically and numerically for various notable network growth models. This section of the chapter is part of an effort of combining information theory with the statistical mechanics treatment of complex network ensembles and a continuation of previous studies assessing the entropy of static networks. Second, we direct our attention to a class of stochastic network growth models that is mostly posed as a candidate mechanism for the neutral evolution of biological networks (protein interaction networks in particular), namely duplication-divergence models. With this class of network growth models in mind, we propose our own version of duplication-divergence models specific to genetic interaction networks and seek to gain an understanding of the recently discovered modularity characteristic of genetic interaction networks called monochromaticity. The dynamics of our stochastic growth models prove to be capable of producing this feature, offering a simplistic yet feasible potential explanation of how that feature might have evolved in nature.
Chapter 3 embodies our contribution to the study of quantum critical phenomena on complex network topologies, which has garnered a great deal of attention in the recent years. It has now been established by statistical physicists working in the field of network science that classical critical phenomena undergo significant changes when dynamical processes take place on complex topologies as opposed to regular networks or lattices. Dynamics of systems governed by quantum mechanical Hamiltonians, however, is a relatively new topic of interest in the network science community. The urgency of the subject of quantum processes on complex topologies has become indubitable as experimental realizations of quantum networks are gradually becoming possible. Here, we are motivated by this trend to ask the question of how quantum phase transitions are affected if they take place on complex networks. To this end, we take two strictly quantum mechanical models and study their phase diagrams for various complex topologies. First, we study the Bose-Hubbard model on annealed and quenched scale-free networks and Apollonian networks. We present our results which reveal the importance of the second moment of the degree distribution and the maximal eigenvalue of the adjacency matrix for the phase diagram of the model. Secondly, we study the phase diagram of the Jaynes-Cummings-Hubbard model on various complex network topologies and demonstrate its dependence on the maximal eigenvalue $\Lambda$ of the hopping matrix and the scaling of $\Lambda$ with the network size $N$.

Interacting multilayered networks represent a relatively recent shift of paradigm in network science bringing the field one step closer to providing a more realistic depiction of interacting complex systems. In Chapter 4, we contribute to the rapidly growing literature on interacting and multiplex networks with an emphasis on the dynamical processes taking place on them. The main question we pose in this chapter is: What are the novel features of dynamical processes – which have otherwise been studied in the context of singular, non-interacting networks – when they are defined on multilayered networks that interact? To this end, we first consider the antagonistic interaction (in other words, competition) between two networks in a simulated setting of a political election campaign. We propose a straightforward mathematical model whereby we model the dynamics of opinion formation through a simulated annealing algorithm and capture the essential features of such a political campaign such as the importance of connectivity and the influence of committed agents, by taking into account the dynamical exchange between the two layers of networks. We then move on to a different dynamical process, the process of centrality ranking, on
multiplex networks. Here we redefine the centrality measure of PageRank for multiplex networks, which we dub “Multiplex PageRank”, which, unlike previous univariate centrality measures, takes into account the connectivity patterns within and across different layers for any multiplex having an arbitrary number of layers. We apply this measure on a real-world multiplex dataset of online communications and find that the ranking with respect to this multiplex centrality measure likely captures elements of the multiplex whose importance is overlooked by the centrality measures defined on single layers.

Continuing in the vein of multiplex and interacting networks, but adding the crucial ingredient of spatial embeddedness, in Chapter 5, we define the statistical mechanics of multiplex and interacting spatial network ensembles. In this chapter, our emphasis is on elucidating the onset of significant link overlap, which is absent in uncorrelated multiplex networks, but experimentally encountered frequently in real-world multiplex network data. Thus, being present in real-world data, we believe that link overlap is an important and defining characteristic worth investigating. We conjecture that the spatial aspect of real-world data introduces correlation to multiplexes, resulting in the emergence of nontrivial link overlap, which we demonstrate analytically with geometric arguments. Not limiting ourselves to multiplexes, we also study interconnected, interacting networks. Here, we approach the subject in a more applied manner and use the dataset of interacting air and railway transportation networks of India to address the topic of navigability from the point of view of a metric modulating the probability of having links between nodes within a certain distance. We show that this link probability metric decays as a power-law for both networks and the bipartite network of interconnections between them, which means that long-distance connections are present in all of them, resulting in improved navigability. This part of the dissertation can be a precedent for future work on transport efficiency from the perspective of statistical mechanics at a time when big data on space and mobility on interacting and multiplex networks is becoming ever more ubiquitous.

We refer the reader to the Background sections of each chapter for a literature review on the respective subjects.

1.1 Some Preliminaries of Network Science

Put in simplest terms, a network is a set of elements with connections between them. The study of networks stems traditionally from a branch of mathematics called graph theory,
which has its roots dating back to the 18th century. The foundations of graph theory were laid by the prolific Swiss mathematician Leonhard Euler when he famously solved the problem of finding a path that traverses each of the seven bridges of Königsberg once and only once. Mathematicians continued to develop graph theory mostly along the lines of regular graphs and trees until the next breakthrough came in the 1950s with the advent of Erdős and Rényi’s random graph theory [15, 16]. Random graph theory, where pairs of vertices are connected uniformly and independently with equal probability, introduced probabilistic methods to the study of graphs, focusing on the statistical properties of networks. The properties of random graphs have been studied rigorously by mathematicians since then, culminating in many important results and proofs.

Meanwhile, another important contribution to network theory came from sociology. In 1967, Stanley Milgram conducted an experiment [17] where he sent packages to a number of people in Nebraska and Kansas, asking them to forward it to someone they knew on a first-name basis whom they believed was more likely to know a “target” contact in Massachusetts. Ideally, each person in this chain forwarded the package until it reached the final destination. Tracking the progress of each chain, Milgram found that the packages that made it to the target had a median chain length of only five acquaintances. This was the first experimental verification of the “small-world” phenomenon, which turned out to be a ubiquitous feature of real-world networks.

In the late 1990s, two groundbreaking publications effectively kickstarted the field of network science, inspired by the proliferation of large real-world datasets. In 1998, Watts and Strogatz proposed the first network model to mimic the small-world behavior and studied it on various real networks [18]. This was followed soon after by Barabási and Albert in 1999 with a network generation model reproducing the hallmark property of power-law degree distribution observed in many real networks [19]. After these, a great amount of interest in complex networks ensued, encouraging people from the fields of physics, computer science, social sciences and biology to go ahead and establish network science as a stand-alone interdisciplinary field.

In the standard nomenclature of graph theory, a graph (network) \( G = (V, E) \) consists of a set \( V \) of vertices (nodes) connected by a set \( E \) of edges (links). Two vertices that have an edge between them are said to be adjacent (neighbors) to each other. The edges in a graph may be undirected or directed. Moreover, the edges may have different weights
represented by real numbers, resulting in a weighted graph. There might be loops (edges that start and end on the same vertex) or multiple edges between the same pair of edges, present in the graph. An undirected, unweighted graph that has no loops or multi-edges is called a simple graph. A graph is connected if there exists a path between any pair of vertices in the graph.

The graph representation that is the most amenable to analytical treatment is the adjacency matrix. For an unweighted graph with \( n \) vertices, the adjacency matrix is an \( n \times n \) matrix \( A \) where the matrix elements \( a_{ij} \) are equal to 1 if there is an edge between vertices \( i \) and \( j \), and 0 otherwise. For undirected networks with no loops, \( A \) is a symmetric matrix, i.e. \( a_{ij} = a_{ji} \), and \( a_{ii} = 0 \). For weighted networks, \( a_{ij} \) is equal to the weight of the edge. The study of the eigenvalues and eigenvectors of the adjacency matrix is an important branch of graph theory called spectral graph theory, which provides important insights into the structural properties of networks.

1.1.1 Structural properties of networks

1.1.1.1 Degree distribution

The most basic property of a node in a network is its degree \( k \), which is the number of links connected to it. In directed networks, nodes are characterized by their in- and out-degrees, meaning the number of incoming and outgoing links, the sum of which gives the number of nearest neighbors of the node. A very important statistical characteristic of networks related to degrees is the degree distribution \( P(k) \), which is the probability of having a uniformly randomly chosen node with degree \( k \). Although degree itself is a local measure, much information can be extracted from the degree distribution about the global organization and structure of a given network.

1.1.1.2 Degree correlations

The degrees of nodes connected by a link are usually correlated in real networks. One of the most useful measures in determining degree correlations in a network is the average degree of the neighbors \( k_{nn}(i) \) of a node \( i \). Moreover, one can define the assortativity \( k_{nn}(k) \) which is the average degree of the neighbors of nodes of degree class \( k \). This measure is indicative of the “mixing patterns” – the systematic tendency of nodes to connect to similar or dissimilar nodes – in a network. If \( k_{nn}(k) \) is increasing with \( k \), the network is said to be assortative with high degree nodes connecting with a higher probability to
other high degree nodes. If \( k_{nn}(k) \) is a decreasing function of \( k \), the network is called *disassortative* meaning that high degree nodes tend to connect to low connectivity nodes and vice versa. Biological and technological networks are mostly disassortative whereas social networks are mostly assortative.

### 1.1.1.3 Clustering coefficient

Introduced originally in sociology under the name *transitivity*, clustering coefficient is an important structural metric that quantifies how cohesive the local neighborhood of a node is. The *local* clustering coefficient \( C_i \) is defined as the ratio of existing links between the neighbors of node \( i \) and the total number of possible links between them. In other words, this is the probability of two neighbors of a node to be neighbors to each other as well, which hints at the tendency of triangles (3-cliques) to form in the network. Averaging the local clustering coefficient over all the nodes of the network gives the *global* clustering coefficient \( C \) of the whole network. One can also define the clustering coefficient \( C(k) \) as a function of degrees, which is informative of how clustering is distributed among different degree classes and can be characteristic for different types of networks.

### 1.1.1.4 Shortest path and diameter

A pair of nodes is connected if there exists a *path* of adjacent nodes between them. In networks, there are usually more than one path connecting two nodes, which lets us define the notion of *shortest path* \( l \) between two nodes. Distance in network terminology is basically the number of links in a path, therefore the shortest path between a given pair of nodes is the one with the smallest distance. One can characterize the size of a network by a related quantity called the *average shortest path* or *diameter* (\( \langle l \rangle \)), which is equal to the shortest paths averaged over all pairs of nodes. For regular lattices of dimension \( d \), this quantity is proportional to \( N^{1/d} \).

### 1.1.1.5 Giant connected component

When the size of the largest connected component in an undirected network approaches a nonzero value as \( N \to \infty \), this cluster becomes a giant connected component (GCC) of the network. In other words, the GCC contains a finite fraction of nodes in an infinite network. For a large enough network, the next largest component is small in size compared to the GCC. The birth of a giant component is the result of the percolation phase transition,
which is a widely studied critical phenomenon defined on complex networks that has been quite revealing about the role of topology in network resilience and robustness.

1.1.1.6 Motifs

Many real-world networks, biological networks in particular [20], contain a small set of recurrent subgraphs called motifs that are over-represented in the network compared to the randomized network with the same degree distribution. They can be interpreted as small circuits that serve as simple building blocks and constitute the network. How significantly they are in the network is usually measured with their normalized Z-score. Different types of networks have different typical motifs that may correspond to certain functions. Moreover, the similarity of the distributions of these motifs in different networks might point towards the presence of underlying processes common to these networks.

1.1.2 The Erdős-Rényi Model

The Erdős-Rényi Model [15, 16], or Poisson random network model, is a very simple yet instructive network model that is frequently used in the study of complex networks. It has been studied rigorously and extensively, and serves as a null model in many situations. There are two variations of the model as proposed originally by Erdős and Rényi, and Gilbert. The $G_{N,p}$ model (sometimes called the Gilbert model [21]) defines the ensemble of all possible graphs consisting of $N$ nodes, where every pair of nodes is connected with a probability $p$. Similarly, the $G_{N,M}$ model defines the ensemble of all possible graphs having $N$ nodes and $M$ uniformly randomly chosen edges. This model of random networks has the small-world property with small average path length $l$, and the degree distribution is Poissonian with $P(k) = (\langle k \rangle)^ke^{\langle k \rangle}/k!$.

1.1.3 Configuration Model

A more generalized form of the random network model is the Configuration Model [22], which creates random networks with a prescribed degree sequence $\vec{k} = k_i$. This method of network generation is useful in that the resultant Poisson degree distribution of the random network model of Erdős and Rényi is not realistic most of the time and other, usually heavy-tailed, degree distributions are desired. The degree sequence $\vec{k}$ can be drawn from any degree distribution $P(k)$, as long as the sum of degrees is even. With the given degree sequence, each node $i$ is assigned $k_i$ “stubs” or half-edges, and then random pairs
of stubs are chosen to be connected until there are no stubs left. This model allows for
the existence of self-loops and multi-edges, although their expected number is vanishingly
small $O(1/N)$ in the large-$N$ limit.

1.1.4 Small-world networks

In their seminal paper, Watts and Strogatz proposed a network model serving as an inter-
mediary between a regular lattice and a random graph [18] which captures both the small
average shortest path length and high clustering coefficient encountered in real networks
by allowing for occasional long-range links in an otherwise ordered network. In this model,
starting from a finite dimensional lattice with periodic boundary conditions (e.g. a ring
lattice), one end of edges are randomly rewired (not allowing for self-links and multi-edges)
with probability $p$, where $p = 0$ corresponds to an intact ring lattice and $p = 1$ corresponds
to a random graph. The average shortest path length scales as $\langle l \rangle \sim \log N$ in small-world
networks. The degree distribution of small-world networks are similar to that of random
networks with a peak at $\langle k \rangle$ decaying exponentially for large $k$.

1.1.5 Preferential attachment: The Barabási-Albert (BA) model

Proposed in 1999 by Barabási and Albert, this model aimed to reproduce the power-law
behavior of the degree distribution in real-world networks by the dynamical process of net-
work growth combined with preferential attachment [19]. Unlike previous models where
the number of nodes $N$ was fixed and the edges were rewired, this model assumed the
addition of nodes one node at a time to an initial collection of $m_0$ nodes. At each step, a
new node is introduced and connected to $m$ ($m \leq m_0$) existing nodes. Furthermore, the
probability of linking the new node to the existing nodes is not equal for all the nodes but
depends on the degree of each node. This “rich get richer” phenomenon is observed in
many real-world networks from citation networks to the World Wide Web. The strength
of the BA model lies in the fact that it’s a dynamical model mimicking the growth of net-
works where the desired topological feature of scale-free degree distribution $P(k) \propto k^{-\gamma}$
arises naturally, yielding a power-law exponent $\gamma = 3$.

Other network growth models inspired by the preferential attachment model have
been proposed over the years, such as the non-linear preferential attachment model of
Krapivsky-Redner-Leyvraz [23, 24], the Bianconi-Barabási model involving the fitness of
nodes [25], Dorogovtsev-Mendes model of initial attractiveness [26] and gradual aging of
nodes [27], etc. A detailed description of these models is provided in Section 2.2.
Chapter 2

The Dynamics of Network Growth

Shedding light on the fundamental rules that govern complex network growth and evolution plays a central role in complex network research. In the past fifteen years, great progress has been made on the modeling of growing social, biological and technological networks. The dynamics of these networks are usually well captured by preferential attachment models or duplication-divergence models that have a hidden effective preferential attachment mechanism. In this chapter, we characterize unexplored aspects of growing network models and their dynamics. First, we define and evaluate the entropy rate, which quantifies the information encoded in growing network models by comparing the number of labeled networks that are typically generated by these dynamic models with the number of static networks with the same degree sequence. Second, we propose epistatic network growth models inspired by the duplication-divergence mechanism to study the roots of monochromaticity in genetic interaction networks.

2.1 Background

Equilibrium networks, where the total number of vertices is fixed, have been the main subject of random graph theory for more than fifty years [15,16]. On the other hand, non-equilibrium or growing networks, where the networks are allowed to grow by the addition of one vertex at a time, have been a relatively recent subject of interest mainly fostered after the empirical discoveries on the inhomogeneous topology of the Internet and other real-world networks [1], especially among the statistical physics community [4]. The most basic non-equilibrium network model is the growing random network model where pairs of vertices to be connected are chosen randomly as the network grows and therefore statistically the oldest vertices are the most connected and the newest vertices are the ones
with the smallest degrees. This causes a departure from the equilibrium configuration of Poisson degree distribution and results in an exponential degree distribution. Likewise, in the more realistic non-equilibrium network growth models with preferential attachment, the most basic version of which is where nodes with a higher degree are preferred to be connected to, the equilibrium is disrupted in favor of the high degree nodes, resulting in a scale-free degree distribution. Examples of growing networks are citation networks [28] where the network continually grows with the addition of new nodes (papers) connected with directed links to (citing) previously published papers; network of collaborations where the network grows as more links (collaborations) are formed between nodes (actors [29], scientists [30], etc.); the World Wide Web [31,32] where the Web grows by the introduction of new nodes (webpages) connecting via directed links (hyperlinks) to others; the Internet [33,34] where the network evolves with the addition of new nodes (servers, clients and routers) and the formation of undirected links (physical wiring) between them. Each type of growing network has its own characteristic pattern of growth, for instance some allow for growing interconnections among old nodes; some do not, due to temporal restrictions.

An important class of growing networks is biological networks. The most studied biological networks include the network of metabolic reactions [35], protein interaction networks [36], ecological and food networks [37, 38] and genetic interaction networks [39]. Stochastic models of network growth such as the duplication-divergence model, detailed in Section 2.3.3 are important to biological networks in that they provide neutral theories for the evolution of these networks. In the neutral evolutionary approach, evolution is considered as an unbiased random walk over all the states of the evolutionary landscape. Within the scope of this thesis, we seek to provide insights into the evolution of a modular structure in genetic interaction networks using neutral network growth models. To serve as a background to this part, we briefly review the literature on genetic interaction networks and their topological properties in Section 2.3.1.

Also of immediate concern to the study of growing networks is the need to quantify the information content of growing network models. In line with this chapter’s emphasis on dynamic growing networks, we take an information theoretic approach and propose entropy measures, namely the entropy rate, for various growing network models. To provide a background to this section of the thesis, we briefly review the literature on entropy measures for complex networks in Section 2.2.1.
2.2 Entropy rate of non-equilibrium growing networks

2.2.1 Complexity measures for networks

The complexity and information content of networks have recently started to be assessed by new entropy measures [40–58]. Being valuable from the theoretical point of view, methods for quantifying complexity may also lead to important applications. This new framework has the potential to resolve one of the outstanding problems in statistical mechanics of complex systems, paving the way for a new information theory of complex network topologies which will provide an evaluation of the information encoded in them.

The entropy of network ensembles quantifies the number of networks with certain structural properties such as degree distribution, degree correlations, community structure or spatial embedding [41–48]. This quantity has been demonstrated to be very instrumental in inference problems defined on networks and it has been successfully applied to the problem of assessing the significance of features for network structure [49]. Other entropy measures of quantum mechanical nature have been derived by mapping the network either to a density matrix or to a quantum state [51–55]. These entropies, defined on single networks, make it possible for the application of quantum information theoretic tools to describe the complexity of single networks and to introduce new kinds of network parameters (for example, by considering the notion of correlations and subsystems). In addition to these measures, the entropy rate of random walks [56–58] is extensively studied on networks, predicting how evenly the random walk spreads in the network. For many applications, it is possible to bias the random walk to construct maximally entropic random walks.

The definitions of entropy of networks introduced above consider static networks hosting dynamical processes. In this part, we define and evaluate the entropy rate of dynamical, growing networks. The literature in the field of growing network models generating scale-free networks is quite extensive [1,4,59–61]. By studying the entropy rate of these models we aim to quantify the number of typical networks that are generated by these models and compare this number to the number of networks that can be constructed with the same degree distribution. We focus particularly on trees to allow for an analytic treatment of the problem. Trees are networks in which cycles are not allowed. The maximal number of possible tree networks generated by a growing network model scales like $N!$ where $N$ is the number of nodes (and links) in the network. The minimal number of tree networks
generated by a growing network model is one, corresponding to the formation of a star or of a linear chain. The entropy rate of growing scale-free networks lies between these two extreme values. Determining the value of the entropy of graphs is informative because it describes the complexity of the growing network models. In fact the value of the entropy will quantify with a unique number the size of the space of typical networks generated by the growing network model. In that regard, the smaller the entropy rate of the networks, the more complex the network structural properties implied by the growing model. In particular, it is essential to determine the scaling of the entropy rate with $N$. Also, in the case where the entropy rate is not constant but depends on $N$, it is important to evaluate the subleading terms that encode for the topology of the networks for other entropy measures as well [42, 43, 54].

Degree correlation is an often used metric in network science. The BA networks are known to have weak degree correlations due to their causal structure. On the other hand, the growing network model with initial attractiveness [26] of the nodes and the fitness model [25] have more significant correlations. To quantify these correlations, different measures have been introduced such as the average nearest neighbor degree or the degree correlation matrix. However, we still lack a way to quantify how much information is encoded in growing network models compared to networks with the same degree distribution constructed by the configuration model.

In this chapter where we focus on growing networks, we aim at quantifying the number of typical tree graphs generated by the non-equilibrium growing network models [19, 23–27, 62] as a proxy of their complexity. This quantity can be used to measure the fraction of networks of a given degree sequence that is generated by growing network models and to quantify in this way the complexity of growing network models. Furthermore, growing network models such as the Bianconi and Barabási fitness model [25, 62] and the non-linear preferential attachment model of Krapivsky and Redner [23, 24], or the growing network model with aging of the nodes [27] are known to undergo structural phase transitions as a function of their parameters. Here we observe that these phase transitions are characterized by a sharp drop of the entropy rate and strong finite-size effects indicating that the network assumes a more ordered state when that threshold is passed.
2.2.2 Gibbs entropy of networks with a given degree distribution

The Gibbs entropy $\Sigma[\{k_i\}]$ [41–45] of a network ensemble with given (graphical) degree sequence $\{k_i\}$ [63, 64] is

$$\Sigma[\{k_i\}] = \frac{1}{N} \log \mathcal{N}[\{k_i\}]$$

(2.1)

where $\mathcal{N}[\{k_i\}]$ is the number of networks with the specified degree sequence and $N$ is the number of labeled nodes $i = 1, 2, \ldots, N$. The Gibbs entropy depends on the number of links but also on the specific details of the degree sequence. In Table 2.1 we give two illustrative examples for two degree sequence compatible with 5 links but defining ensembles of networks with different entropy.

<table>
<thead>
<tr>
<th>Degree Sequence</th>
<th>Networks</th>
<th>Entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,1,1,1,5</td>
<td><img src="image1.png" alt="Network" /></td>
<td>$\Sigma[{k_i}] = 0$</td>
</tr>
<tr>
<td>1,2,2,2,3</td>
<td><img src="image2.png" alt="Network" /></td>
<td>$\Sigma[{k_i}] \neq 0$</td>
</tr>
</tbody>
</table>

Table 2.1: The configuration of networks with degree sequence $\{1,1,1,1,5\}$ (on top, $\mathcal{N}[\{k_i\}] = 1$) and $\{1,2,2,2,3\}$ (on bottom, $\mathcal{N}[\{k_i\}] = 6$).

It turns out that the ensemble of networks having a given degree distribution is a type of microcanonical network ensemble satisfying a large number of hard constraints (the degree of each node is fixed). It is also possible to construct canonical network ensembles similar to what happens in classical statistical mechanics when one distinguishes the microcanonical and canonical ensembles according to the fact that the energy is perfectly conserved or conserved in average. A canonical network ensemble with given expected degree sequence is an ensemble of graphs in which the degree of each node is distributed as a Poisson variable with given expected degree $\{\bar{k}_i\}$. The entropy of the canonical network ensemble is the logarithm of the typical number of networks in the ensemble. This
entropy $S[[k_i]]$ is given by

$$S[[k_i]] = -\frac{1}{N} \left[ \sum_{ij} p_{ij} \log p_{ij} - \sum_{ij} (1 - p_{ij}) \log (1 - p_{ij}) \right]$$

(2.2)

where $p_{ij}$ indicates the probability that a node $i$ is linked to a node $j$. We can evaluate the entropy of a maximally random network ensemble with given expected degree distribution $\{k_i\}$ by maximizing the entropy $S[[k_i]]$ with respect to $p_{ij}$ under the conditions

$$k_i = \sum_j p_{ij}.$$  

(2.3)

In this way we get for the marginal probabilities $p_{ij}$ [44]

$$p_{ij} = \frac{\theta_i \theta_j}{1 + \theta_i \theta_j},$$

(2.4)

where $\theta_i$ are related to the Lagrangian multipliers, or “hidden variables” fixed by the constraints given by Eqs. (2.3). In particular, for the uncorrelated network model in which $\overline{k}_i < \sqrt{\langle k \rangle N}$ and $p_{ij} = \frac{k_i k_j}{\langle k \rangle N}$, the Shannon entropy network ensemble takes a direct form [43]

$$S[[k_i]] = \frac{1}{2} \langle k \rangle [\log(\langle k \rangle N) - 1] - \frac{1}{N} \sum_i (\ln \overline{k}_i - 1) \overline{k}_i.$$  

(2.5)

The Gibbs entropy $\Sigma$ of a microcanonical ensemble of networks with degree sequence $\{k_i\}$ with $k_i = \overline{k}_i$ is given by [45]

$$\Sigma\{k_i\} = S\{k_i\} - \Omega\{k_i\}$$

(2.6)

where $\Omega\{k_i\}$ is the entropy of large deviations of the canonical ensemble

$$\Omega\{k_i\} = -\frac{1}{N} \log(\sum_{a_{ij}} p_{ij}^{a_{ij}} (1 - p_{ij})^{1-a_{ij}} \prod_i \delta(\sum_j a_{ij}, k_i)).$$

(2.7)

where $\{a_{ij}\}$ is the adjacency matrix of the network. In particular the matrix element $a_{ij}$ of the adjacency matrix is given by $a_{ij} = 1$ if a link is present between node $i$ and node $j$ while $a_{ij} = 0$ otherwise. By replica methods and the cavity method [42, 45] it is possible
to derive the given expression for $\Omega \{ k_i \}$,

$$\Omega \{ k_i \} = -\frac{1}{N} \sum_i \log \pi_{k_i}(k_i), \quad (2.8)$$

where $\pi_r(n)$ is the Poisson distribution with $\langle n \rangle = r$. In particular, for the uncorrelated network model in which $k_i < \sqrt{\langle k \rangle N}$ and $p_{ij} = \frac{k_i k_j}{\langle k \rangle N}$, the Gibbs entropy network ensemble takes a direct form [43]

$$\Sigma \{ k_i \} = \frac{1}{2} \langle k \rangle \log(\langle k \rangle N) - 1 - \frac{1}{N} \sum_i \left( \ln k_i - 1 \right) k_i +$$

$$- \frac{1}{2N} \sum_i \log(2\pi k_i) - \frac{1}{4N} \left( \frac{\langle k^2 \rangle}{\langle k \rangle} \right)^2. \quad (2.9)$$

We might as well define the Gibbs entropy $\Sigma \{ N_k \}$ of networks with given degree distribution $\{ N_k \}$. Since the number of graphs with given degree distribution $\mathcal{N}\{ N_k \}$ is just given by

$$\mathcal{N}\{ N_k \} = \mathcal{N}\{ k_i \} \frac{N!}{\prod_k N_k!} \quad (2.10)$$

it follows that

$$\Sigma \{ N_k \} = \Sigma \{ k_i \} - \sum_k \frac{N_k}{N} \log \left( \frac{N_k}{N} \right). \quad (2.11)$$

### 2.2.3 Entropy rate of growing trees

Many networks are non static but they are growing by the addition of new nodes and links. A major class of growing networks are growing trees in which at each time a new node and a new link is added to the network. In the last ten years, many growing network models have been proposed. Special attention has been addressed to growing network models generating scale-free networks. In fact these stylized models explain the basic mechanism according to which many growing natural networks develop the universally found scale free degree distribution. The fundamental model for scale-free growing network is the BA model [19] which generates networks with degree distribution $P(k) \sim k^{-\gamma}$ and $\gamma = 3$. This model is based of two ingredients: growth of the network and preferential attachment meaning that nodes with large degree are more likely to acquire new links. Here we consider this model and other different significant variations to this model including different additional mechanisms as initial attractiveness of the nodes [26], fitness of the nodes [25,62], non-linear preferential attachment [23,24] and aging of the nodes [27]. Some
of these models as explained below undergo structural phase transitions to be studied by statistical mechanics methods.

2.2.3.1 Growing network models

In the growing scale-free network model we start from two nodes linked together, at each time $t = 1, 2, \ldots$

- we add a new node $i = t + 2$;
- we link the new node to a node $i_t$ of the network chosen with probability

$$\Pi(i_t) = \frac{A_i}{\mathcal{N}},$$

where $\mathcal{N} = \sum_{i=1}^{t+1} A_i$;
- the number of nodes in the network is $N = t + 2$.

As a function of the choice of $A_j$ different networks model are defined. In particular we consider the following growing network models:

- If we take $A_i = \delta_{i,1}$, we get a star graph;
- If we take $A_i = \delta_{i,t+1}$, we get the linear chain;
- If we take $A_i = 1$, we get a maximally random connected and growing tree;
- If we take $A_i = k_i$, where $k_i$ is the degree of the node $i$, we get the BA model [19];
- If we take $A_i = k_i - 1 + a$, with $a < 1$, we get a generalized BA model with initial attractiveness of the nodes [26];
- If we assign to each node a fitness value $\eta_i$ from a distribution $\rho(\eta) = 1$ and $\eta \in (0, 1)$ and we take $A_i = \eta_i k_i$, we get the Bianconi-Barabási fitness model [25].
- If we take $A_i = k_i^{\gamma'}$, we get the non-linear preferential attachment model of Krapivsky-Redner [23, 24]. This network model undergoes a gelation phenomenon for $\gamma' > 1$. Namely, there is an emergence of a single dominant node linked to almost every other node. For $\gamma' > 2$, there is a finite probability that the dominating node is the first node of the network.
If we assign to each node a fitness value \( \eta_i = e^{-\beta \epsilon_i} \), with \( \epsilon_i \) drawn from a distribution \( g(\epsilon) \propto \epsilon^\kappa \) and \( \kappa > 0 \), and we take \( A_i = \eta_i k_i \), we get as a function of \( \beta \) the so called "Bose-Einstein condensation in complex networks" of Bianconi and Barabási [62]. When this happens, for \( \beta > \beta_c \) one node with high fitness is connected to a finite fraction of other nodes in the network.

If we take \( A_i = (t - t_i)^{-\alpha} k_i \) where \( t_i \) indicates the time at which the node \( i \) has joined the network, we get the preferential attachment model with aging of the sites of Dorogovtsev-Mendes [27]. In this growing network the power-law exponent \( \gamma \) of the degree distribution is diverging as \( \gamma \approx \frac{1}{c_1} \frac{1}{1-\alpha} \) when \( \alpha \to 1^- \). For \( \alpha > 1 \) the network is exponential and becomes more and more similar to a linear chain.

### 2.2.3.2 Entropy rate

The growing connected trees are fully determined by the sequence of symbol \( X = (i_1, i_2, \ldots, i_N) \) where \( i_t \) is the node linked at time \( t \) to the node \( i = t + 2 \). In order to evaluate the entropy rate of growing networks it is sufficient to determine the entropy rate of the sequence \( (i_1, i_2, \ldots, i_t) \):

\[
h(t, X) = - \sum_{i_t} P(i_t | i_1, i_2, \ldots, i_{t-1}) \log P(i_t | i_1, i_2, \ldots, i_{t-1}),
\]

(2.13)

where \( P(i_t | i_1, i_2, \ldots, i_{t-1}) \) is the conditional probability that the node \( i_t \) is chosen at time \( t \) given the history of the process. The entropy of the process evaluating how many networks are typically constructed by the growing network process is \( S(\{X\}) \):

\[
S(\{X\}) = - \sum_{\{i_1, i_2, \ldots, i_t\}} P(i_1, i_2, \ldots, i_t) \log P(i_1, i_2, \ldots, i_t).
\]

(2.14)

### 2.2.3.3 Maximal and minimal bound to the entropy rate of growing network trees

It is instructive to study the limits of the entropy rate of connected growing trees. The minimal entropy rate is given by the entropy rate of the star or of the linear chain. Indeed by taking \( A_i = \delta_{1,i} \) we have that the entropy rate is zero. Indeed the growing network model becomes deterministic and it gives rise to a unique star network with the center on the node \( i = 1 \). The entropy rate of a linear chain \( A_i = \delta_{i,t+1} \) is also zero by a similar argument and the model generates a unique linear chain network structure. On the other
hand the maximal entropy rate is given by the maximally random growing connected trees that is generated by taking $A_i = 1$ and $\Pi_i = 1/(t + 1)$. For this process the entropy rate is given by

$$h(t, \mathcal{X}) = \log(t + 1)$$

(2.15)

Therefore this entropy rate increases logarithmically with time and the probability of each tree with $N = t + 2$ nodes is given by

$$P(N) = \frac{1}{(N - 1)!}$$

(2.16)

Therefore $S(\{\mathcal{X}\}) = \log[(N - 1)!]$. This is the maximal entropy of a growing connected tree.

### 2.2.4 Growing trees with stationary degree distribution

For growing network models with stationary degree distributions there are simple relations between $h(t, \mathcal{X})$ and $S(\{\mathcal{X}\})$. Indeed let us define the entropy rate

$$H(\mathcal{X}) = \lim_{N \to \infty} \frac{1}{N} [S(\{\mathcal{X}\}) - \log((N - 1)!)]$$

(2.17)

For a growing tree network with stationary degree distribution, by the recursive application of chain rule $P(i_1, i_2, \ldots, i_t) = P(i_t|i_1, i_2, \ldots, i_{t-1})P(i_1, i_2, \ldots, i_{t-1})$ we can easily get

$$H(\mathcal{X}) = \lim_{N \to \infty} \frac{1}{N} \left[ \sum_{n=1}^{N-2} h(n, \mathcal{X}) - \log((N - 1)!)] \right.$$

(2.18)

If the entropy rate of growing networks $H$ is a constant, it means that the number of graphs generated by the growing network model has a dominating term which goes like $N!$ and a subleading term that is exponential with the number of nodes $N$. On the contrary if $H = -\infty$ it means that the number of networks generated by the growing network model increases with the number of nodes in the network $N$ at most exponentially. Usually the typical number of labeled networks generated by growing network models with convergent degree distribution is less than the number of networks with the same degree distribution. In order to evaluate the ratio between these two cardinalities, we introduce here the difference $\Delta$ between the Gibbs entropy $\Sigma\{\{N_k\}\} of the network with the same degree distribution and the entropy of the networks generated by the growing network model.
Therefore $\Delta$ is
\[
\Delta = \lim_{N \to \infty} \left\{ \Sigma\{N_k\} - \frac{1}{N} \log[(N - 1)!] - H(\mathcal{X}) \right\}.
\] (2.19)

The larger the value of $\Delta$ is, the smaller the fraction of networks generated by the growing model compared with the networks generated by the configuration model. This implies that the larger is $\Delta$ the more complex the networks generated by the growing models are. In fact these networks need the dynamics of the networks implicitly force the networks to satisfy more stringent set of structural conditions beyond the degree distribution.

2.2.4.1 The entropy rate of the BA model

We consider the BA model, we take $A_i = k_i$ and $\Pi_i = \frac{k_i}{2(N-1)}$ therefore
\[
P(i_t|i_1, i_2, \ldots, i_{t-1}) = \frac{k_t}{2(N-1)}.
\] (2.20)

The BA model, asymptotically in time has a degree distribution that converges to the value $N_k$ given by
\[
N_k = \frac{4N}{k(k+1)(k+2)}.
\] (2.21)

Therefore, asymptotically in time the entropy rate of the BA model is
\[
h(t = N - 2, \mathcal{X}) \to -\sum_{k=1}^{\infty} N_k \frac{k}{2(N-1)} \log \left( \frac{k}{2(N-1)} \right).
\] (2.22)

Hence, the entropy rate $h(\mathcal{X})$ increases in time as the logarithm of the number of nodes in the network, but it has a subleading term which is constant in time and depends on the degree sequence, i.e.
\[
h(t = N - 2, \mathcal{X}) \to \log(N - 1) + \log(2)
- \sum_{k=1}^{N-1} \log(k) \frac{2}{(k+1)(k+2)}
\to \log(N - 1) - 0.51(0)
\] (2.23)

The entropy rate $H(\mathcal{X})$ in the limit $N \to \infty$ is therefore given by
\[
H(\mathcal{X}) \simeq -0.51 \ldots
\] (2.24)

We note here that the degree distribution $N_k$ is known to have interesting finite size...
effects [4,65], in addition to the asymptotic scaling Eq.(2.21). Here we checked that the value of the entropy rate is not modified by these corrections up to the significant digit we have considered. Finally, in order to compare the number of networks generated by the BA model with the network that we can construct with the same degree sequence, we evaluate the value of $\Delta$ in the thermodynamic limit. This can be written as

$$
\Delta = \lim_{N \to \infty} \left\{ \frac{1}{N} \sum_{t=1}^{N-1} \log(N/t) \right. \\
- \frac{1}{2N} \sum_{k} N_k [k \log(k) + \log(2\pi k)] \\
- \sum_{k} \frac{N_k}{N} \log \left( \frac{N_k}{N} \right) + 1 \left\} \right. \\
\simeq 0.9(1) \quad (2.25)
$$

2.2.4.2 The entropy rate of the growing network model with initial attractiveness

If we take $A_i = k_i - 1 + a$, the network generated is scale free with power-law exponent $\gamma = 2 + a$ [26]. The probability to choose the node $i_t$ given the history of the process is therefore given by

$$
P(i_t|i_1, i_2, \ldots, i_{t-1}) = \frac{A_i}{N} = \frac{k_i - 1 + a}{(a + 1)(N - 1)}. \quad (2.26)
$$

Asymptotically in time the degree distribution for trees converges to the value [4,26]

$$
N_k = N(1 + a) \frac{\Gamma(1+2a)\Gamma(k+a-1)}{\Gamma(a)\Gamma(k+1+2a)}. \quad (2.27)
$$

From this, the entropy rate $h(t, X)$ is asymptotically

$$
h(t = N - 2, X) \to \\
- \sum_{k=1}^{\infty} N_k \frac{k - 1 + a}{(a + 1)(N - 1)} \log \left[ \frac{k - 1 + a}{(a + 1)(N - 1)} \right], \quad (2.28)
$$
which can be simplified as
\[
h(t = N - 2, \mathcal{X}) \rightarrow \log(N - 1) + \log(a + 1) \\
- \sum_{k=1}^{N-1} \log \left[ (k - 1 + a) \frac{\Gamma(1 + 2a)\Gamma(k + a)}{\Gamma(a)\Gamma(k + 1 + 2a)} \right]. \]
(2.29)

In the limit \( N \to \infty \), the entropy rate \( H(\mathcal{X}) \) is
\[
H(\mathcal{X}) = \log(a + 1) \\
- \sum_{k=1}^{N-1} \log \left[ (k - 1 + a) \frac{\Gamma(1 + 2a)\Gamma(k + a)}{\Gamma(a)\Gamma(k + 1 + 2a)} \right]. \]
(2.30)

When \( a \to 1 \), the solution reduces to the solution of the BA model. In Fig. 2.1 we plot the value of \( H = H(\mathcal{X}) \) versus \( a \) calculated by Eq. (2.30) using an upper cutoff for the degree \( k_i < K \forall i = 1, \ldots N \). As the parameter \( a \to 0 \) the entropy rate decreases indicating that the network model generates an exponentially smaller number of networks. Also the Gibbs entropy of scale free networks decreases as long as the power-law exponent converges toward 2, i.e. in the limit \( \gamma \to 2 \). In order to evaluate the change in the ratio of networks generated by the growing network model to the number of possible networks with the same degree distribution, in Fig. 2.2 we plotted \( \Delta \) as a function of \( a \). As \( a \to 0 \) and \( \gamma \to 2 \) the number of networks generated by the growing network models are a smaller function of the total number of networks that is possible to build with the same degree distribution. This is an indication and quantification of the importance of correlations generated by the growing network model with given initial attractiveness \( a \).

### 2.2.4.3 The entropy rate of the Bianconi-Barabási fitness model

If the kernel \( A_i \) is heterogeneous and specifically given by \( A_i = \eta_i k_i \), the model is called Bianconi-Barabási fitness model [25]. The probability to choose the node \( i_t \) given the history of the process is therefore given by
\[
P(i_t|i_1, i_2, \ldots, i_{t-1}) = \frac{A_i}{N} = \frac{\eta_i k_i}{\mu(N - 1)}, \]
(2.31)
Figure 2.1: The entropy rate $H$ calculated for the growing network model with initial attractiveness [26] as a function of $a$ and evaluated by Eq. (2.30) using a maximal degree equal to $K = 10^7$.

Figure 2.2: The value of $\Delta$ calculated for the growing network model with initial attractiveness [26] as a function of $a$ evaluated for networks of $N = 50000$ nodes and over 20 realizations of the process.
where \( \mu(N - 1) = \sum_{i=1}^{N-1} \eta_i k_i \). The degree distribution \( N_k(\eta) \) for nodes of fitness \( \eta \), asymptotically in time converges to [61]

\[
N_k(\eta) = \frac{N \mu \rho(\eta) \Gamma(k) \Gamma(1 + \mu/\eta)}{\eta \Gamma(k + 1 + \mu/\eta)},
\]

(2.32)

where \( \rho(\eta) \) is the distribution of \( \eta \). Given the analytic solution of the model [25, 61], \( \mu \) is determined by the self-consistent relation

\[
\int_0^{\rho_0} \rho(\eta)(\mu/\eta - 1)^{-1} d\eta = 1
\]

(2.33)

We consider here the case of uniform distribution of the fitness, i.e., \( \rho(\eta) = 1 \) with \( \eta \in (0, 1) \). Therefore the entropy rate is given by

\[
h(t = N - 2, \mathcal{X}) \rightarrow
- \sum_{k=1}^{N-1} \int_0^1 N_k(\eta) \frac{\eta^k}{\mu(N - 1)} \log \left( \frac{\eta^k}{\mu(N - 1)} \right),
\]

(2.34)

which gives

\[
H(\mathcal{X}) = -1.59\ldots
\]

(2.35)

2.2.4.4 Entropy rate for growing network models with structural phase transitions

We have measured the entropy rate for three growing network models showing a phase transition:

- The Krapivsky-Redner model [23, 24] with

\[
h(t, \mathcal{X}) = -\sum_{i=1}^{t} \frac{k_i^\gamma}{\mathcal{N}} \log \left( \frac{k_i^\gamma}{\mathcal{N}} \right)
\]

and \( \mathcal{N} = \sum_{i=1}^{t} k_i^\gamma \)

- The Bianconi-Barabási model showing a Bose-Einstein condensation in complex networks [62] with

\[
h(t, \mathcal{X}) = -\sum_{i_t} e^{-\beta \epsilon_i} k_i \log \left( \frac{e^{-\beta \epsilon_i} k_i}{\mathcal{N}} \right)
\]

and \( \mathcal{N} = \sum_{i_t} e^{-\beta \epsilon_i} k_i \).
The Dorogovtsev-Mendes model with aging of the nodes \[27\] with

\[
h(t, \mathcal{X}) = -\sum_{i} \frac{\tau_i^{-\alpha} k_i}{N} \log \left( \frac{\tau_i^{-\alpha} k_i}{N} \right)
\]  

(2.38)

where \( \tau_i = t - t_i \) is the age of node \( i \) and \( N = \sum_{i=1}^{t} \tau_i^{-\alpha} k_i \).

In Fig. 2.3 the entropy rate \( H(\mathcal{X}) \) is calculated by numerical simulations using

\[
H(\mathcal{X}) = \frac{1}{N} \left[ \sum_{n=1}^{N-2} h(n, \mathcal{X}) - \log((N - 1)!) \right].
\]  

(2.39)

for a network of sufficiently large size \( N \) for the three models as a function of the parameters \( \gamma, \beta \) and \( \alpha \) respectively. We show that at the transition point the scaling of \( H \) evaluated for a network of size \( N \) changes from constant to an \( N \) dependent behavior. In particular we checked that in the three cases \( H \propto \log(N) \) indicating that as the network grows the typical number of networks that are generated scales only exponentially with \( N \) (and not like \( N! \)).

This behavior signifies a disordered-ordered phase-transition in the topology of the network. In the Bose-Einstein condensation network model and in the Krapivsky-Redner model, below the phase transition, the network is dominated by a hub node that grabs a finite fraction of the nodes. In the aging model, below the phase transition, the network develops a structure more similar to a linear chain.

### 2.2.5 Concluding Remarks

In this section of the thesis, we have studied growing network models and their entropy rate. The entropy rate allows us to calculate the number of typical graphs generated by growing scale-free network models and to quantify their complexity by comparing this number to the total number of graphs with the same degree distribution. We have studied the entropy rate of scale-free tree networks, and we have seen that the entropy rate of growing simple trees have maximal and minimal bounds. Our focus was on trees but the definition of entropy rate can be easily extended to growing network models with cycles. However the probabilities of adding two or more links at a given time should explicitly account for the fact that the new links must be distinct, a fact which induces a small correction to the simple preferential attachment. We have also studied non-equilibrium growing network models showing structural phase transitions. By numerical investigations,
Figure 2.3: The entropy rate $H$ is evaluated for the Kapivsky-Redner model [23,24] (panel A), for the "Bose-Einstein condensation in complex networks" of Bianconi-Barabási with $g(\epsilon) = 2\epsilon$, and $\epsilon \in (0,1)$, $(\kappa = 1)$ [62] (panel B) and for the aging model [27] of Dorogovtsev-Mendes (panel C). The data are averaged over $N_{\text{run}}$ different realizations of the network. We took $N_{\text{run}} = 100$ for simulations with $N = 10^4$ and $N_{\text{run}} = 30$ otherwise. Above the structural phase transition indicated with the solid line, the entropy rate $H$ strongly depends on $N$. 

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we have shown that when a growing network model has a phase transition, the entropy rate changes its scaling with the system size, indicating the disorder-to-order transition. In the future, we believe that an integrated view of information theory of complex networks will provide a framework to extend quantitative measures of complexity to a large variety of network structures, models and dynamics. The work presented in this thesis is a step in this direction.

2.3 Monochromaticity in Neutral Evolutionary Network Models

2.3.1 Modularity in genetic interaction networks

Highly interacting molecular networks [20, 66–71] are at the forefront of systems biology and are essential to understand biological systems beyond the single molecule framework. Among the research on biological networks, a recent focus has been on the study of complex genetic interactions [72, 73]. This interest is mainly due to the fact that the relationship between phenotypes and genotypes is inherently a complex one – phenotypes are most commonly determined by simultaneous interactions between multiple genes rather than by a single gene [74]. These genetic interactions are furthermore complicated by the fact that the effects of individual genes are modified by other genes, resulting in the phenomenon called epistasis. The epistatic network between mutations or genetic variations in the genome is found to play a crucial role in determining the fitness of different organisms [72, 73]. This network is interacting with the other biological networks of the cell such as the protein-protein interaction network [36, 75] the metabolic network [35] or the transcription network [71, 76] and is crucial in determining the phenotype of an organism. The degree distribution of these networks is clearly fat-tailed [73] thus showing a similar topology with respect to other biological networks. Moreover the genes involved in epistatic interactions can have a hierarchical relationship; they can mask or modify each other’s effects and even combine to create new phenotypes.

Biological systems are also known to often display a functionally modular architecture on various levels [77]. In biological networks, a modular topology [20, 78] is usually predictive of the presence of functional modules and therefore topological considerations [79, 80] have relevance in detecting the function and dynamics of these networks. Much of the robustness and adaptability of biological networks has been attributed to this modular
structure. Modularity in biological networks has been studied from the perspectives of topology [78], information theory [81] and more recently, epistasis.

A recent study [72] has investigated epistasis through a genetic interaction network constructed by the calculation of epistasis values $\epsilon$ from the fitnesses of all of the single and double knockouts of 890 metabolic genes of Saccharomyces Cerevisiae (budding yeast). In both supervised organization with known gene annotations and unsupervised organization with unknown gene functions, the study revealed a structural clusterability into modules that interact with each other monochromatically, that is, via the same type of epistasis. Monochromaticity in the interactions between functional modules was later verified as part of a genome-wide genetic interaction study [73] of Saccharomyces Cerevisiae. In this larger scale research, the genetic interaction map of the budding yeast was constructed from 5.4 million gene pairs. Modules belonging to different pathways and complexes were shown to be interacting via the same type of epistasis almost exclusively. Most recently, there have been efforts in introducing measures to quantify monochromaticity [82, 83].

The origin of the functional modularity is not thoroughly characterized: at first it was considered to be due to evolutionary pressure [20] but more recently observations have shown that modularity might be the natural outcome of neutral evolution [84]. In the third section on this chapter, in line with our focus on dynamical network growth mechanisms, we will seek to elucidate the evolutionary origin of modularity and clusterability in epistatic networks to see if it can be described as the product of a stochastic network growth process. The stochastic growth models that are used as well as the so called Duplication-Divergence mechanism they are modeled after are described in detail in Section 2.3.3.

In this section, we ask how the monochromaticity feature emerged in nature. We want to gain insight into whether it can be explained as the outcome of a neutral evolutionary theory, driven by stochastic processes. To this end we devise network models inspired by the duplication-divergence model [85–88] that is shown to successfully capture the heterogeneous network properties and other important topological features of protein interaction networks. Focusing on the genomic level, we propose neutral evolutionary models in which epistatic networks of genes are constructed via similar duplication-divergence processes for the epistatic interaction signs. Signs of links are copied as genes are duplicated and they
are switched and/or rewired with finite probability. We generate ensembles of epistatic networks using these models and assess their monochromaticity using the PRISM algorithm [72] which makes use of agglomerative clustering to detect modules. The number of monochromaticity violations $Q_{\text{module}}$ of these networks are compared to their randomized versions where the topology is preserved and the epistatic signs are shuffled. We show that the $Q_{\text{module}}$ distribution for epistatic network ensembles generated by these models are centered around zero indicating monochromaticity, and are statistically significantly different from their randomized counterparts, which are not monochromatic. In particular, the last model that we propose in which we assume epistasis between genes that encode proteins belonging to protein complexes, displays a clear separation of its conflict number distribution from that of the randomized ones and is strictly monochromatic. The degree distributions of each of these models display a fat tailed behavior, with the degree distributions of positive and negative interactions showing no deviation from each other as there is no bias towards any sign in any of the models.

### 2.3.2 Epistasis: The multiplicative model

A mathematical definition of epistasis that was introduced by population geneticists in order to deal with complex traits such as human diseases in a quantitative and statistical way is known as the multiplicative model. Widely used in genetic interaction studies, it makes use of the quantitative measure $\epsilon$ which is the difference between the fitness $W_{AB}$ of a double mutant and the product of fitnesses of two single mutants $W_A, W_B$, i.e.

$$\epsilon = W_{AB} - W_A W_B$$

The sign of this deviation from multiplicative behavior helps distinguish between two different classes of interactions: a positive (antagonistic) epistasis signifies a buffering type of interaction in which the effect of the double mutation is less severe than single mutations combined; a negative (synergistic) epistasis means an aggravating type of interaction where the double mutation results in a more severe effect on the fitness.

### 2.3.3 Duplication-Divergence Mechanism

Gene duplication and the subsequent mutations (divergence) is believed to be one of the most crucial mechanisms driving evolution [89]. In the past decade, mathematical models that make use of the duplication-divergence mechanism have been proposed and studied analytically [85–88]. These models were successful in capturing the basic topological prop-
erties of protein interaction networks such as scale-free degree distribution, small-world properties, modular architecture and robustness against random node removal. The duplication parts of these models are carried out in a similar way to each other. First, a random gene is selected to be duplicated, which is called a target gene. The duplicated new gene then acquires all of the interactions of the target gene. This makes sense in the proteomic viewpoint as the interactions of proteins are determined by their structure, which remains unchanged after duplication. The divergence part, on the other hand, is model specific and shows some variation from model to model in terms of the exact divergence mechanism. Usually, what is understood by divergence is the removal of interactions with some finite probability. Duplication-divergence models are divided into two classes according to the link removal mechanism. In asymmetric models [85,90] only the duplicated genes can lose links whereas in symmetric duplication-divergence models [86], both the original and duplicated genes can lose their interactions. In some of the duplication-divergence models, this removal can be accompanied by rewiring of the links or formation of new links with some other finite probability.

In this thesis we implement three epistatic network models based on the duplication-divergence mechanism with additional focus on the interaction signs. The epistatic interactions are mediated by protein interaction networks. Therefore a duplication-divergence model for the evolution of epistatic interactions implements a minimal hypothesis on their dynamical evolution. We start from a simple initial condition common to all of the three models. During the duplication phase, the interaction type is preserved whereas in the case of rewiring, the epistatic signs of the new links are chosen as detailed in the following subsections for each model.

2.3.4 Monochromaticity

The monochromaticity – the feature of clusterability into modules that interact via the same type of epistasis – of each model is studied using the PRISM algorithm [72], which was originally developed to study the yeast metabolic network. Belonging to a class of hierarchical clustering methods known as agglomerative clustering, the algorithm starts out with each element in a cluster of its own. It assigns a conflict score $C_{x,y}$ to every cluster pair $(x,y)$, which is total number of “mixed sign” or nonmonochromatic links and then at each step determines the set of cluster pairs with the minimum conflict score

$$C_m = \min_{x,y} \{C_{x,y}\}$$
It then selects from this set the one pair of clusters with the highest proximity (determined by the density of links between them) and combines them. This process is repeated until the whole network is covered. Finally, a total monochromaticity violation number $Q_{\text{module}}$ which is the sum of the minimum conflict scores over all the steps

$$Q_{\text{module}} = \sum C_m$$

is assigned to the final clustering solution. A total conflict number of zero means a fully monochromatic solution. The result of this analysis on the yeast metabolic network reported in [72] is that the unsupervised organization of the real yeast metabolic network yielded a fully monochromatic solution. Unsupervised in this context means having no prior knowledge of the genes’ functional annotations. Moreover, this unsupervised organization of the epistatic network resulted in modules that agree well with existing gene annotations. A supervised version of this analysis was also carried out in this study for pre-assigned functional annotation groups, which also yielded a statistically significant enrichment of monochromatic interactions.

### 2.3.5 Monochromaticity in Duplication-Divergence Inspired Epistatic Models

In this section we take a similar approach in which we investigate the distributions of the total conflict score $Q_{\text{module}}$ for the networks constructed by duplication-divergence models and their randomized counterparts. The color randomization scheme consists of the pairwise flipping of signs so that the topology of the network is preserved as well as the total number of positive and negative interactions. Following the unsupervised approach, we don’t make any assumptions as to the function of genes. Since the duplication-divergence models are themselves of stochastic nature, we represent their total conflict score as a distribution as well.

#### 2.3.5.1 Model A

The first model that we consider for the neutral evolution of epistatic networks is a simple generalization of the model introduced by Solé et al. [85]. The Solé model is one of the first models to be developed as a growing network model to simulate proteome evolution. It has two free parameters $\delta$ and $\alpha$ which are the probability of removal of the links of the duplicated gene and the probability of the duplicated gene to form links with any of the previously unlinked genes, respectively. It was shown to successfully capture
structural properties of the yeast proteome such as the degree distribution [85], sparse nature and modularity [91]. Here we generalize this model in order to capture a simple neutral evolution of the epistatic network. We start with simple initial conditions: at the beginning the network is initialized with three nodes and two links so that $E_{12} = 1$ and $E_{13} = -1$ where $E$ is the interaction matrix composed of the elements $-1$ (negative epistasis), $1$ (positive epistasis) and $0$ (no interaction). The epistatic implementation of this model for a network size of $n$ consists of the iteration of the following set of rules (Fig. 2.4).

Figure 2.4: Duplication-Divergence scheme of the Model A. The target node is indicated by the small arrow and the duplicate node is in grey. Green (light grey) links denote positive interactions and red (dark grey) links negative interactions. Interactions are duplicated with the same signs; removed (dashed lines) with probability $\delta$ and linked (dotted lines) to previous nodes with random signs with probability $\alpha$.

(i) **duplication:** A target node $v_i \in V$ is chosen at random and the replicated node $v_r = v_{n+1}$ acquires all the links $\{e_{i,j}\}$ of the target node where $\{v_j\}$ is the set of neighbors of $v_i$. The signs are copied during duplication so that $E_{rj} = E_{ij}$.

(ii) **divergence 1 (deletion):** Each of the links $e_{r,j}$ of the replicated node is deleted with probability $\delta$.

(iii) **divergence 2 (addition of new links):** The replicated node $v_r$ is connected with a random sign to all of the previously unconnected nodes with probability $\alpha$, which is typically a small number.

The parameters used in this work, namely $\delta = 0.5$ and $\alpha = 0.0002$ were chosen so that they are compatible with the estimated average connectivity from mean-field calculations [85].
and experimental data.

An instance of the epistatic network generated by Model A is shown in Fig. 2.5. The total degree distribution and sign degree distributions (Fig. 2.6) of this model both display fat tailed distributions with an exponential cutoff although it is easy to disrupt the power law distribution of this model by increasing the rewiring probability, in which case the distribution becomes exponential similar to that of a random growing network. Furthermore, both positive and negative interaction degree distributions follow the same trend as there is no bias in the model towards any sign.

Figure 2.5: A sample network given by the model A for $\delta = 0.5$ and $\alpha = 0.0002$. Positive and negative links are denoted by green (light grey) and red (dark grey) links, respectively.

The distribution of the total number of conflicts of the networks generated by Model A and their random counterparts is shown in Fig. 2.7. To get this distribution, a total number of 100 networks were generated and subsequently randomized. The resulting histogram shows a clear separation of the means in the duplication-divergence ensemble (shown in black) and randomized ensemble (shown in white). The conflict score of model A is very close to zero ($0.91 \pm 1.45$) whereas the corresponding randomized distribution has much larger spread. To test for the null hypothesis that the means of the distributions are the same, or in other words the null assumption that the expected $Q_{\text{module}}$ is given by the randomized network, we ran a statistical significance test on the distributions, which yielded a p-value of $8.43 \times 10^{-25}$, which means that the distributions are statistically signif-
icantly different, with model A giving a monochromatic solution whereas the randomized version isn’t.

2.3.5.2 Model B

In Model A the epistatic interactions of different signs remain strongly localized in different regions of the network as it appears clearly in the graphical representation of the network (Fig. 2.5). In this section we provide a first modification of the model which has the effect of maintaining the fat-tail degree distribution while at the same time mixing further the epistatic interactions of different signs. Model B has two free parameters and takes into account the probability to connect to one of the second neighbors of the target node in the case of removal of the duplicated node. The duplication (i) step is the same as in the previous model whereas the divergence is different. Here in the following we give the precise definition of the algorithm we have implemented for Model B. The iterative steps are summarized in Figure 2.8. We start with the same initial conditions as in model A, i.e. we start with three nodes and two links such that the epistatic interactions are given by $E_{12} = 1$ and $E_{13} = -1$ where $E$ indicates the sign of the epistatic interaction.

(i) duplication: A target node $v_i \in V$ is chosen at random and the replicated node $v_r = v_{n+1}$ acquires all the links $\{e_{i,j}\}$ of the target node where $\{v_j\}$ is the set of neighbors of $v_i$. The signs are copied during duplication so that $E_{rj} = E_{ij}$.

(ii) divergence 1 (deletion): Each of the links $e_{r,j}$ of the replicated node is deleted with probability $p$. 

Figure 2.6: The total (left) and sign (right) degree distributions of the model A for $\delta = 0.5$ and $\alpha = 0.0002$. Circles and triangles denote negative and positive links, respectively.
Figure 2.7: The total monochromaticity violation number $Q_{\text{module}}$ distributions of model A networks (black) and their randomized counterparts (white) for 100 realizations of each. The parameters used are $\delta = 0.5$ and $\alpha = 0.0002$.

(iii) **divergence 2 (rewiring):** The replicated node $v_r$ is connected to one of the second neighbors of the target node with probability $q$ in the case of removal of the duplicated link. The sign of the rewired link to the second neighbor is the product of the signs of the first and second neighbors such that $E_{rk} = E_{ij} \times E_{jk}$.

This model suggests that when a gene is duplicated, newly emerging epistatic interactions follow a transitive sign rule (divergence 2 mechanism). Although epistatic interactions are known to be non-linear and in general a transitivity of the sign might not be the rule, it is possible that for epistatic interactions mediated by protein-interaction networks this mechanism for divergence might effectively take place. A sample network generated by Model B is given in (Fig. 2.9). The free parameters for this model were chosen as $p = 0.4$ and $q = 0.01$ for removal and rewiring, respectively. Here the network has a more mixed topology due to the rewiring to the second neighbors, therefore the monochromatically clusterable architecture is not evident from the figure of the network. Still, the scale free degree distribution is preserved (Fig. 2.10) as the rewiring is made with only one of the second neighbors of the target node, per removal of the duplicate link. Positive and negative degree distributions are again indiscernible.

Duplication-divergence model B and randomized networks have the $Q_{\text{module}}$ distribution as shown in (Fig. 2.11). An ensemble of 100 networks was used to collect statistics on
Figure 2.8: Duplication-Divergence scheme of model B. The target node is indicated by the small arrow and the duplicate node is in grey. Green (light grey) links denote positive interactions and red (dark grey) links negative interactions. Interactions are duplicated with the same signs; removed (dashed lines) with probability $p$ and in the case of removal, rewired to one of the second neighbors of the target node with probability $q$ according to the sign convention described below.

Figure 2.9: A sample network given by model B for $p = 0.4$ and $q = 0.01$. Positive and negative links are denoted by green (light grey) and red (dark grey) links, respectively.

monochromaticity for this model. In Figure 2.11 the total conflict distribution of model B is presented and it appears as slightly more spread than Model A although it is still centered close to zero ($3.83 \pm 4.36$). The corresponding randomized distribution is also
Figure 2.10: The total (left) and sign (right) degree distributions of model B for $p = 0.4$ and $q = 0.01$. Circles and triangles denote negative and positive links, respectively.

more separated ($61.41 \pm 53.22$). The p-value under the same null hypothesis as the Model A is $1.26 \times 10^{-21}$. This also complies with the results above, indicating monochromatic separability of model B.

2.3.5.3 Model C

This model is a generalization of the basic model which preserves the fat-tail degree distribution and implies a well-mixed distribution of epistatic interactions with different signs. The model is a very stylized one that takes into account the functional dependencies of protein complexes on each other. In this model, we assume that a duplicated gene might encode a protein that belongs to a protein complex which is either the same complex as that of the template protein (gene) or a complex that competes with the original template gene by aggravating interactions. Genes encoding proteins in competing protein complexes have aggravating (negative) interactions between them, pointing to a redundancy in the essential cellular functions of the two complexes. On the other hand, genes encoding proteins in the same complex have alleviating interactions between them. [92,93]. In Figure 2.12 we give a schematic view of the two different possibilities that are contemplated in this model.

We start with the same initial conditions as in model A and B, i.e. we start with three nodes and two links such that the epistatic interactions are given by $E_{12} = 1$ and $E_{13} = -1$ where $E$ indicates the sign of the epistatic interaction. At each iteration we perform the subsequent steps (Fig. 2.13):

(i) duplication: A new duplicated node $v_r = v_{n+1}$ is a gene that encodes for a protein
in the same complex \((E_{ri} = 1)\) or in a competing complex \((E_{ri} = -1)\) with respect to that of a randomly chosen template node \(v_i \in V\) with equal probability. If the replicated gene encodes for a protein in the same complex, the replicated node acquires all the links \(\{e_{i,j}\}\) of the target node with the same sign, i.e. \(E_{rj} = E_{ij}\). If the replicated gene encodes for a protein that belongs to a competing complex, the replicated node acquires all the links \(\{e_{i,j}\}\) of the target node with the opposite sign, i.e. \(E_{rj} = -E_{ij}\).

(ii) **divergence (deletion):** Each of the links \(e_{r,j}\) of the replicated node is deleted with probability \(p\).

A typical network constructed by Model C is shown in (Fig. 2.15). The only free parameter is the probability of removal of the duplicated links, which is chosen to be \(p = 0.6\). The epistatic signs are thoroughly mixed in this network, due to the equally probable assignment of positive and negative interactions between the target node and the duplicated node, and the ensuing sign convention of the duplicated links. This model permits the generation of two types of triangular motifs, namely pnn and ppp triangles (Fig. 2.14) where p and n indicate respectively positive (buffering) and negative (aggravating) interactions. The underlying protein complex assumption is supported by the findings that pnn triangle motifs are encountered mostly between protein complexes separated by a negative
Figure 2.12: Schematic view of protein complexes and their epistatic interactions. A duplicated gene (D) can encode for a protein in the same protein complex as the template gene (T) (Panel (a)), or belong to a competing protein complex (Panel (b)). The figure shows the epistatic interactions in both cases.

edge suggesting a supportive coordination of function between them [92, 93].

The degree distributions of this model are fat tailed as well despite the presence of some skewness in the power law distribution. The degree distributions of interactions with different signs follow the same trend (Fig. 2.16).

An ensemble of 150 networks was used for the total conflict distribution. Compared to the other two models, this model is much more defined in terms of monochromaticity and gives a fully monochromatic solution (Fig. 2.17). The separation of the duplication divergence model from its randomized counterpart ($80.16 \pm 18.80$) is apparent.

2.3.6 Concluding Remarks

In this section, we have investigated the modular structure and monochromatic clusterability of epistatic networks generated using stochastic models inspired by the duplication-
Figure 2.13: Duplication-Divergence scheme of model C. The template node is indicated by the small arrow and the duplicate node is in grey. With equal probability (1/2) the duplicated gene encodes for a protein in the same complex (double green (light grey) link) or in a competing complex (double red (dark grey) link) with respect to the protein encoded by the target gene. Signs of the duplicated links are chosen according to the definition of the model. Removed interactions (with probability p) are shown by dashed lines.

Figure 2.14: The two triangular motifs generated by model C. Positive and negative links are denoted by green (light grey) and red (dark grey) links, respectively.

... divergence method in order to test for a neutral evolutionary hypothesis. We have shown that these genetic interaction networks have total monochromatic violation score distributions that are close to zero and are statistically significantly different from their randomized counterparts. This fact implies that these networks comply with the monochromaticity feature observed in real genetic interaction data of model organisms such as the budding yeast.

Overall, the investigation of models based on the duplication-divergence mechanism is a good first step toward understanding the evolutionary origins of monochromaticity although it is important to stress that these mathematical models are very simplistic and further investigation into real biological networks is called for to extract information about what features are more relevant to monochromaticity in order to be able to tweak the details of these models. The parameter space of the three proposed models were explored before the $Q_{module}$ distributions were plotted and the free parameters were chosen so as to...
Figure 2.15: A sample network given by model C for $p = 0.6$. Positive and negative links are denoted by green (light grey) and red (dark grey) links, respectively.

Figure 2.16: The total (left) and sign (right) degree distributions of model C for $p = 0.6$. Circles and triangles denote negative and positive links, respectively.

reproduce the general topological properties (scale-free degree distribution, average connectivity) of model organisms. Therefore it is fair to say that the results presented in this study constitute a snapshot of the models since modularity comes about in a relatively narrow range of parameters. Duplication-divergence does not account for the preference of these specific parameters. It is likely that they might be the result of some selection for sparse graphs in nature [94]. So biological modularity cannot be explained solely by natural selection or neutral evolution but rather as the result of contributions from both
Figure 2.17: The total monochromaticity violation number $Q_{\text{module}}$ distributions of model C networks (black) and their randomized counterparts (white) for 150 realizations of each. The parameter is chosen as $p = 0.6$

– an example being neutral mechanisms such as duplication-divergence whose parameters are tweaked by natural selection. The same is most likely valid for monochromaticity. In fact it is difficult to say that neutral evolution is the only explanation underlying it, although our findings with duplication-divergence models do corroborate its role.

One possible future direction to take, as far as assessing what the relevant structural characteristics in real biological networks are, would be to do a motif significance investigation on real data. Motifs are highly represented subgraphs in networks that occur statistically more frequently than they should in the randomized counterparts of networks [95]. Although the immediate functional significance of individual motifs has been a disputed topic, it is still informative about the network structure. Interesting parallels might be drawn between the motifs of real networks and implemented mathematical models. Model C in particular calls for such an analysis for different triangle types (4 overall). A comparison between these particular motifs in the yeast interaction network and networks generated by Model C can help improve the already promising ability of this model to reproduce monochromaticity in a biologically motivated way. An important point to note is that Model C as it is presented in this work can produce two out of the four possible triangle motifs due to transitivity of signs. The two remaining motifs that are not produced by this model, namely nmn and ppp triangles, are mainly associated with
synthetic lethal interactions and biochemical pathways, respectively [93]. Exploring the monochromaticity of models that result in these motifs might provide a more complete picture of the monochromaticity phenomenon in a wider scope of biological interactions.
Chapter 3

Dynamical Quantum Processes on Complex Topologies

The last decade has seen important advances in the study of classical critical phenomena such as the classical Ising model and the percolation transition on complex networks. It has been revealed that the existence of complex network topologies can significantly alter the phase diagrams of critical dynamical processes unfolding on these networks. The behavior of quantum critical phenomena on complex topologies, however, has recently begun to be investigated. As part of this effort, we direct our attention in this chapter to the dynamics of systems defined by two quantum mechanical models, namely the Bose-Hubbard model and the Jaynes-Cummings-Hubbard model. We first characterize the phase diagram of the Bose-Hubbard model by mean-field approximation on annealed and quenched scale-free networks. Next, we investigate the phase diagram of the Jaynes-Cummings-Hubbard model and characterize the Mott-insulator to superfluid phase transition on a number of topologies through both analytical and numerical approaches.

3.1 Background

Critical phenomena unfolding on complex networks has been a recent focus of research [5, 6]. It has been observed that the topology of networks might significantly change the phase diagram of dynamical processes. As an example of this, the Ising model [96–99], the percolation phase transition [100, 101] and the epidemic spreading dynamics on annealed networks [102] are strongly affected when networks have a scale-free degree distribution $P(k) \sim k^{-\lambda}$ and the second moment $\langle k^2 \rangle$ diverges with the network size, in other words
when $\lambda \in (2, 3]$. Moreover, epidemic spreading on quenched networks [103, 104], synchronization stability [105, 106], critical behavior of $O(N)$ models [107, 108] and critical fluctuations of the Ising model on spatial scale-free networks [109] are all driven by the spectral properties of networks.

Quantum critical phenomena might also depend on the topology of the underlying lattice as it has been shown for Bose-Einstein condensation in heterogeneous networks [110]. Although the attention has been mainly on classical critical phenomena on scale-free networks, the behavior of quantum critical phenomena on scale-free networks has recently begun to be investigated. To this end, the Anderson localization [111, 112] was studied in complex networks showing that by modulating the clustering coefficient of the network one might induce localization transition in scale-free networks. Moreover, quantum processes on Apollonian networks – an example of scale-free networks embedded in two dimensions – have been studied [113, 114], showing that the maximal eigenvalue of the adjacency matrix diverges with the network size. The quantum processes investigated on Apollonian networks are the Hubbard model [115], the free electron gas within the tight-binding model [116], and the topology induced Bose-Einstein condensation [117]. Particularly in recent years, the study of quantum phase transitions on these networks has attracted attention, motivated by the creation of a new self-similar macromolecule – a nanometer-scale Sierpinski hexagonal gasket [118]. Recently [119] it has been shown that the Random Transverse Ising model is strongly affected by a scale-free network topology of the underlying networks on which it is defined, especially by the second moment of the degree distribution $\langle k^2 \rangle$. Indeed the critical temperature for the onset of the disordered phase is infinite if this second moment diverges and the network is scale-free with power-law exponent $\lambda \leq 3$.

Meanwhile, research at the interface of quantum information and complex networks has also gained considerable momentum in the past few years. The potential realization of quantum networks with complex topologies made possible by the effective long-range interactions between fiber-coupled optical cavities [120–122] has brought these fields together. Among studies conducted in this vein are quantum ranking and navigation algorithms for complex topologies [123, 124], dissipative continuous-time quantum walks on complex networks [125] and the use of entanglement entropy to quantify the mutual information on complex quantum networks [126].
3.2 Bose-Hubbard Model on Complex Networks

Here we investigate the dynamics of the Bose-Hubbard model [127–130] – a critical process with no classical equivalent – on complex networks, particularly on scale-free topologies. In the current framework of ultracold atom physics, defect free potentials have been constructed and the phenomenology of systems described by the Bose-Hubbard model experimentally reproduced [131]. By superimposing different lattices with incommensurate lattice constants, disordered systems of ultracold atoms have recently been experimentally investigated [132]. As the experimental technology advances, it might become possible to investigate the role of topological network complexity in the phase diagram of the Bose-Hubbard model. Moreover, this complex topology might be effectively present in complex granular materials and might affect insulator-superconductor phase transitions [133] in these systems. Hence, a full account of the consequence of complex topologies might turn out to shed some light on the phase diagram of these complex materials. In fact the model defined on complex networks might provide a useful mean-field approximation to real disordered granular materials that captures essential features of their heterogeneity. Finally the Hubbard model is a theoretical model that has applications far beyond condensed matter physics [134, 135] and investigating its properties on scale-free networks might stimulate further applications to other fields. Different approaches have recently been suggested for the theoretical study of the Bose-Hubbard model. Here we cite field theoretic approximations [128, 136–138], mean-field approximations, [129, 130, 139, 140], quantum Monte Carlo simulations [141–146], and quantum cavity methods [147], among many others.

In this section, we show by mean-field approximations that the phase diagram of the model defined on an annealed network depends on the second moment of the degree distribution $\langle k^2 \rangle$. In particular, by the mean-field approximation, we find both for annealed and quenched networks that for scale-free networks with $\lambda \leq 3$, the Mott insulator phase reduces with increasing network size, disappearing in the thermodynamic limit. Furthermore, we observe differences between the model defined on quenched networks and annealed networks. In fact, it is sufficient for a quenched random network to have diverging maximum degree in order to reduce the Mott-insulator phase to zero in the thermodynamic limit. This demonstrates that complex networks might strongly perturb the phase diagram of quantum phase transitions.
3.2.1 The Bose-Hubbard Model

The Bose-Hubbard model is described by the Hamiltonian

$$\hat{H} = \sum_i \frac{U}{2} n_i(n_i - 1) - \mu n_i - t \sum_{i,j} \tau_{ij} a_i a_j^\dagger$$

(3.1)

where the indices $i, j = 1, \ldots N$ indicate the nodes of the network. The network has an adjacency matrix $\tau$ such that $\tau_{ij} = 1$ if there is a link between node $i$ and node $j$, otherwise $\tau_{ij} = 0$. The operator $a_i^\dagger(a_i)$ creates (annihilates) a boson at site $i$ and $n_i = a_i^\dagger a_i$ counts the bosons at site $i$. The parameter $U$ represents the repulsive boson-boson interaction, $t$ represents the hopping amplitude between neighboring nodes while $\mu$ indicates the chemical potential. The hallmark of this Hamiltonian is a quantum phase transition between the Mott insulating phase and the superfluid phase originating from the competition between the kinetic and the repulsive terms of the Hamiltonian. Strictly speaking, the Mott insulating phase with vanishing compressibility is present only at zero temperature. At finite temperature, thermal fluctuations induce a phase transition between the superfluid phase and the normal phase.

3.2.2 Mean-field solution of the Bose-Hubbard Model on annealed complex networks

Annealed networks evolve dynamically over the same time scale as the dynamical process occurring on it. During this process, links are created and annihilated but the expected degree of each node remains the same. We consider the ensemble of uncorrelated networks in which we assign to each node a hidden variable $\theta_i$ from a distribution $p(\theta)$, indicating the expected number of neighbors of a node. The probability to draw a link between node $i$ and $j$ is given by $p_{ij}$

$$p_{ij} = P(\tau_{ij} = 1) = \frac{\theta_i \theta_j}{\langle \theta \rangle N}.$$  

(3.2)

In this ensemble the degree $k_i$ of a node $i$ is a Poisson random variable with expected degree $\overline{k_i} = \theta_i$. Therefore we will have

$$\langle \theta \rangle = \overline{\langle k \rangle}$$

and

$$\langle \theta^2 \rangle = \overline{\langle k(k - 1) \rangle}.$$  

(3.3)

where $\langle \ldots \rangle$ indicates the average over the $N$ nodes of the network and the overline in Eq. (3.3) indicates the average over the ensemble of the networks. We assume that the
expected degree distribution of the network ensemble is given by

\[ p(\theta) = N \theta^{-\lambda} e^{-\theta/\xi} \] (3.4)

where \( N \) is a normalization constant and \( \xi \) is an exponential cut-off in the expected degree distribution.

In order to study the Bose-Hubbard model on annealed complex networks we consider the fully connected Hamiltonian given by

\[ H = \sum_i \frac{U}{2} n_i (n_i - 1) - \mu n_i - t \sum_{i,j} p_{ij} a_i a_j^\dagger. \] (3.5)

where in order to account for the dynamical nature of the annealed graph we have substituted the adjacency matrix element \( \tau_{ij} \) in \( H \) given by Eq. 3.1 with the matrix element \( p_{ij} \) given by Eq. 3.2.

We perform the mean-field approximation to the Bose-Hubbard model introduced in [139] by taking

\[ a_i a_j^\dagger \simeq \langle a_i \rangle a_j^\dagger + a_i \langle a_j^\dagger \rangle - \langle a_i \rangle \langle a_j^\dagger \rangle \]

\[ \simeq \psi_i a_j^\dagger + a_i \psi_j - \psi_i \psi_j \] (3.6)

where \( \psi_i = \langle a_i \rangle = \langle a_i^\dagger \rangle \). The Hamiltonian is then decomposed in single site terms

\[ H = \sum_i H_i + \langle \theta \rangle N t \gamma^2 \] (3.7)

with \( H_i \) given by

\[ H_i = \frac{U}{2} n_i (n_i - 1) - \mu n_i - t \theta_i \gamma (a_i + a_i^\dagger) \] (3.8)

where \( \gamma \) indicates the order parameter of the superfluid phase, defined as

\[ \gamma = \frac{1}{\langle \theta \rangle N} \sum_i \theta_i \psi_i. \] (3.9)

Therefore in this mean-field picture the Hamiltonian decouples into single site (node) Hamiltonians \( H_i \) depending on the mean-field order parameter \( \gamma \). We can write the single site (node) Hamiltonian as an unperturbed Hamiltonian plus an interaction depending on
the parameter $\gamma$, i.e.

$$H_i = H_i^{(0)} + \gamma \theta_i V_i$$

(3.10)

with

$$H_i^{(0)} = \frac{U}{2} n_i (n_i - 1) - \mu n_i$$

$$V_i = t(a_i + a_i^\dagger)$$

(3.11)

The ground state energy $E_i^{(0)}(n) = E^{(0)}(n)$ with $E^{(0)}(n^*) = 0$ if $\mu < 0$ and $E^{(0)}(n^*) = -\mu n^* + \frac{1}{2} U n^*(n^* - 1)$ if $\mu \in (U(n^* - 1), U n^*)$. The second order correction to the energy is given by $E_i^{(2)}(n^*)$

$$E_i^{(2)}(n^*) = \gamma^2 t^2 \theta_i^2 \sum_{n \neq n^*} \frac{|\langle n| V_i | n^* \rangle|^2}{E^{(0)}(n^*) - E^{(0)}(n)}$$

$$= \gamma^2 t^2 \theta_i^2 \left( \frac{n^*}{U(n^* - 1) - \mu} + \frac{n^* + 1}{\mu - Un^*} \right)$$

Therefore the energy spectrum $E$ is given by the eigenvalues of the Hamiltonian $H$ Eq. (3.8), i.e.

$$E = \text{const} + m^2 \gamma^2$$

(3.12)

with

$$m^2 \frac{\langle \theta^2 \rangle}{t \langle \theta \rangle N} = 1 + t \frac{\langle \theta^2 \rangle}{\langle \theta \rangle} \left( \frac{n^*}{U(n^* - 1) - \mu} + \frac{n^* + 1}{\mu - Un^*} \right).$$

(3.13)

The phase transition between a Mott-insulator phase where $\gamma = 0$ and a superfluid phase where $\gamma > 0$ occurs when $m = 0$. Therefore the phase diagram at $T = 0$ is given by

$$t_c(U, \mu, T = 0) = U \frac{\langle \theta \rangle}{\langle \theta^2 \rangle} \left( \frac{\mu/U - n^*}{(n^* - 1) - \mu/U} \right)$$

(3.14)

with $\mu/U \in [n^* - 1, n^*]$. The difference with respect to the mean-field phase diagram for regular lattices is that $t_c$, the critical hopping rate, depends on the second moment of the expected degree distribution, i.e. $\langle \theta^2 \rangle = \langle k(k - 1) \rangle$. Given the general expression for the expected degree distribution of the networks considered in this section, i.e. Eq. 3.4 including the exponential cut-off $\xi$, the Mott-insulator phase disappears as $\xi \to \infty$ when $\lambda \leq 3$ and remains finite if $\xi \to \infty$ and $\lambda > 3$. Therefore as $\frac{\langle \theta^2 \rangle}{\langle \theta \rangle}$ diverges i.e. as $\xi \to \infty$ while $\lambda \leq 3$, we have that the Mott insulator phase shrinks and finally disappears for large network sizes. Also it can be seen that the critical indices will deviate from the mean-field
values and they can be found by applying the heterogeneous mean-field techniques [99] developed for the classical phase transition.

At finite temperatures, we cannot properly speak of a Mott insulator phase but we still have a phase transition between the normal phase and the superfluid phase. The local order parameter is given by the thermal average of the creation and annihilation operators, i.e.

\[
\psi_i = \frac{\text{Tr } a_i e^{-\beta H_i}}{\text{Tr } e^{-\beta H_i}}.
\]

(3.15)

Following the same steps as in [129], we can prove that the critical line for the Mott insulator, superfluid phase is given by

\[
t_C(U, \mu, \beta) = \frac{\langle \theta \rangle}{\langle \theta^2 \rangle} \frac{\sum_r e^{\beta [\mu r - (U/2) r (r-1)]}}{\sum_r Q_r(U, \mu) e^{\beta [\mu r - (U/2) r (r-1)]}}.
\]

(3.16)

where

\[
Q_r(U, \mu) = \frac{\mu + U}{(\mu - Ur)(U(r - 1) - \mu)}.
\]

(3.17)

Therefore the phase diagram at finite temperature is also affected by the topology of the network and significantly changes when \(\langle \theta^2 \rangle\) diverges.

### 3.2.3 Phase diagram of the Bose-Hubbard Model on quenched complex networks

Here we discuss the phase diagram of the Bose-Hubbard model on quenched networks, whose structure does not change in time. In particular we focus on the phase diagram at \(T = 0\). The Hamiltonian we consider is the original Bose-Hubbard Hamiltonian defined on the adjacency matrix \(\tau\) (Eq. 3.1). Once again, we solve this equation in the mean-field approximation assuming Eq. (3.6) and \(\psi_i = \langle a_i \rangle = \langle a_i^\dagger \rangle\). By solving self-consistently for \(\psi_i\) we find the boundary of the Mott-insulator phase where \(\psi_i = 0\) and the superfluid phase where \(\psi_i > 0 \forall i\). The mean-field Hamiltonian \(H^{MF}\) is then parametrized by the self-consistent parameters \(\psi_i\) and reads

\[
H^{MF} = \sum_i \left[ \frac{U}{2} n_i(n_i - 1) - \mu n_i - t \sum_j \tau_{ij}(a_i + a_i^\dagger) \psi_j \right] + t \sum_i \sum_j \tau_{ij} \psi_i \psi_j.
\]

(3.18)
Following [130] we consider the hopping term as a perturbation. At the first order of the perturbation theory we get that

$$\psi_i = t \frac{\partial}{\partial \mu} F(\mu, U) \sum_j \tau_{ij} \psi_j$$

(3.19)

where

$$F(\mu, U) = \frac{\mu + U}{[\mu - n^* U][U(n^* - 1) - \mu]}$$

(3.20)

and $\mu \in (U(n^* - 1), Un^*)$. Therefore, if $\Lambda$ is the maximal eigenvalue of the adjacency matrix $\{\tau_{ij}\}$, the Mott insulator phase with $\psi_i = 0$ is stable provided that

$$\frac{t}{U} F(\mu, U) \Lambda < 1.$$  

(3.21)

It is observed that in random scale-free networks with degree distribution $p(k) = Nk^{-\lambda}$, the maximal eigenvalue $\Lambda$ of the adjacency matrix diverges with a diverging value of the maximal degree of the network $k_{max}$ as $\Lambda \propto \sqrt{k_{max}}$ [148–151]. In line with this, we also find that as long as the maximal degree of the network diverges, the Mott insulator phase disappears in the large network limit, changing the phase diagram of the model significantly with respect to regular networks where the maximal degree of the network remains constant. We check the validity of these results by performing numerical integration of the mean-field calculations. We study the phase diagram of single quenched networks with scale-free degree distribution $p(k) = Nk^{-\lambda}$ and different values of the power-law exponent $\lambda$ to see how fast the convergence of the solution to the asymptotic phase diagram is.

In the following we show our finite-size scaling calculations and the resulting effective phase diagram of the Bose-Hubbard model within the mean-field approximation on the quenched network for different values of the number of nodes $N$. In (figure 3.1) we plot the effective phase diagram for network sizes $N = 100, 1000, 10000$, finding that for $\lambda = 2.2 < 3$ the boundary of the Mott insulating phase decreases with the network size. On the other hand for a typical network with $\lambda = 3.5 > 3$ (see figure 3.2) the phase diagram has slower finite size dependencies.

This, together with the results from the previous section, shows that the annealed approximation for the Bose-Hubbard model on scale-free networks differs strongly from the quenched phase diagram of the model for $\gamma > 3$. In particular we have that the Mott insulator phase transition on annealed scale-free networks, with diverging second
Figure 3.1: Average order parameter for the superfluid phase for scale-free networks with power-law exponent $\lambda = 2.2$ and network sizes $N = 100$ (top) $N = 1000$ (middle) and $N = 10,000$ (bottom). As the network size increases the phase diagram changes monotonically as predicted by the mean-field treatment in the case $\lambda < 3$. Therefore there is no Mott-insulator phase in the limit $N \to \infty$. 

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Figure 3.2: Average order parameter for the superfluid phase for scale-free networks with power-law exponent $\lambda = 3.5$ and network sizes $N = 100$, $N = 1000$ and $N = 10,000$. As the network size increases the phase diagram has slower finite size effects with respect to the case $\lambda < 3$. Nevertheless the maximal eigenvalue increases with network size as $\Lambda \propto \sqrt{k_{\max}}$ and therefore the Mott insulator phase disappears in the thermodynamic limit in this case as well.
moment of the degree distribution, vanishes in the thermodynamic limit while in quenched networks it is sufficient that the most connected node has a diverging connectivity in the thermodynamic limit to destroy the Mott insulator phase.

3.2.4 Phase diagram of the Bose-Hubbard Model on Apollonian networks

In this section, we study the phase diagram as predicted by the mean-field approximation, on Apollonian networks [113]. Apollonian networks are an example of scale-free networks embedded in a two-dimensional space. They are constructed by considering the classical 2D Apollonian packing model in which the space between three tangent circles placed on the vertices of an equilateral triangle is filled by a maximal circle. The space-filling procedure is repeated for every space bounded by three of the previously drawn tangent circles. The corresponding Apollonian network is constructed by connecting the centers of all the touching circles (Fig. 3.3 (left)). The resulting network is scale-free with power-law degree distribution \( p(k) = N k^{-\lambda} \) and \( \lambda = 1 + \ln(3)/\ln(2) \approx 2.585 \). These networks are also known to have diverging maximal eigenvalue \( \Lambda \) of their adjacency matrix [114]. Therefore, our expectation is that the Mott insulator phase of the Bose-Hubbard model should also disappear in the large network limit in these networks. We use the iterative scheme introduced in [114] to generate 5th (Fig. 3.3 (right)), 7th and 9th generation Apollonian networks, where the number of nodes in the \( n \)th generation is \( N(n) = (3^n + 5)/2 \). In Fig. 3.4 we demonstrate the finite-size effects on the phase diagram found in the mean-field approximation.
Figure 3.4: Effective phase diagram of the Bose-Hubbard model on Apollonian networks of the 5th, 7th and 9th generation, with network sizes $N = 124$, $N = 1096$ and $N = 9844$, respectively. As the network size diverges the Mott-Insulator phase is reduced and it disappears in the limit of an infinite network.

We note here that in experimental realizations of the Bose-Hubbard model on Apollonian networks it might be relevant to include a hopping term that also depends on the distance between the nodes. The dynamics on this weighted network might further modify the phase diagram of the process. In this section, we have chosen to study the simple case in which the hopping doesn’t depend on the distance, leaving the characterization of the dynamics on the weighted network for future investigations.

3.2.5 Concluding Remarks

In this part of the thesis, we have demonstrated that the scale-free network topology of the underlying network strongly affects the phase diagram of the Bose-Hubbard model. We have performed mean-field calculations on annealed networks and studied the phase diagram of the model both at $T = 0$ and at finite temperature, showing that the Mott insulator phase disappears in the large network limit as long as the power-law exponent $\lambda$
of the degree distribution is $\lambda \leq 3$ and the exponential cutoff $\xi$ of the distribution diverges. Moreover, the analytical and numerical solutions of the Bose-Hubbard model on quenched networks show that this argument must be corrected in the quenched case and that it is sufficient that the maximal eigenvalue diverges in order to change the phase diagram of the model. Finally we have considered the Bose-Hubbard model on Apollonian networks that are an example of scale-free networks embedded in a two dimensional space. In summary, this work offers a new perspective on the characterization of quantum critical phenomena on annealed and quenched complex networks and shows that the second moment of the degree distribution $\langle k^2 \rangle$ and the maximal eigenvalue of the adjacency matrix play a crucial role in determining the phase diagram of the Bose-Hubbard model.

3.3 Jaynes-Cummings-Hubbard Model on Complex Networks

3.3.1 Light-matter interactions on complex topologies

Recent advances in quantum optics and atomic physics have allowed for an unprecedented level of control over light-matter interactions which not only makes the emulation of condensed matter models feasible [152,153], but also inspires new architectures conceiving a future quantum Internet with a desired topology [120,154]. The potential advantage coming from a combined optical and atomic approach is twofold: on one hand, being able to control a quantum system that simulates another one is a way to realize a special purpose quantum computer; on the other hand, the possibility of manipulating new degrees of freedom not accessible in condensed matter systems motivates the experimental and theoretical study of new quantum systems, with the possibility of discovering new physical phenomena. In this respect, an important result coming from the combined experimental investigations of atomic and optical systems is the realization of coupled cavity arrays interacting with local atomic degrees of freedom [152]. These systems permit the controlled interaction between trapped atoms and local cavity photons and moreover, photons are free to hop between coupled cavities. By changing the details of the physical setup, different many-body models can be realized [152,155], and one in particular is of interest to this chapter: the Jaynes-Cummings-Hubbard (JCH) model [156–162]. Part of the interest in these systems is motivated by the possibility to investigate new quantum critical phenomena [127] such as the quantum phase transition of light between a Mott-like regime and a superfluid phase [156–162]. Also of interest is the possibility to generate quantum simulators that naturally access non-equilibrium physics [163].
The additional degree of freedom which optical arrays can provide, in other words, the topology of the network underlying the quantum dynamics, is the main focus of this section. While regular lattice structures with short-range interactions are the typical framework in standard quantum emulator architectures, fiber-coupled cavities may allow for the realization of quantum networks with distant effective interactions between local degrees of freedom [120–122]. These effective long-range interactions are an important ingredient for the construction of quantum networks with complex topology, which is a recent topic of interest in the quantum information and complex network community [10, 54, 55, 110–112, 115–117, 119, 123–126, 164]. Along this line of research, we study in this section the effect of the array topology on the phase diagram of the JCH model. Motivations come from the possible experimental realization of such systems, as well as a number of results highlighting the importance of networks’ topologies. Indeed for classical systems it is well known that the topology of the network can significantly change the phase diagram of some models, and their critical behavior [5, 6]. On the quantum side previous results on the Bose-Hubbard model [128–132] are particularly inspiring for the present work. In fact, for this model, it has been shown by mean-field arguments that the phase diagram depends of the maximal eigenvalue \( \Lambda \) of the hopping matrix describing the topology of the network [10, 130]. This result is valid both in the presence of disorder [130] and in the presence of a complex topology [10] (see also Section 3.2).

In this part, we investigate the properties of the JCH model on complex network topologies. Using mean-field theory we characterize the phase diagram of the model at \( T = 0 \), which presents a phase transition between a Mott-like regime and a superfluid phase. We demonstrate analytically and confirm numerically that the phase diagram is non-trivial and well defined only if the hopping coefficient \( \kappa \) scales as the inverse of the maximal eigenvalue \( \Lambda \) of the hopping matrix, i.e. \( \kappa \propto \frac{1}{\Lambda} \). Furthermore, we characterize the scaling of the maximal eigenvalue for a number of well known complex network topologies, showing that in many cases the maximal eigenvalue \( \Lambda \) diverges with the network size \( N \). Therefore our results are of general interest for a number of different complex topologies, and they imply that interesting quantum critical behavior can be observed in complex network arrays, even with very small couplings between different cavities.
3.3.2 Jaynes-Cummings model: Atom-photon interaction in a single cavity

The Jaynes-Cummings Hamiltonian provides the standard model describing the interaction between a two-level atom and quantized electromagnetic modes. In the rotating wave approximation, and assuming a single cavity mode, the Hamiltonian is given by

\[ H_{JC} = \epsilon \sigma^+ \sigma^- + \omega a\dagger a + \beta (\sigma^+ a + \sigma^- a\dagger) \] (3.22)

where \( \epsilon \) is the atomic transition frequency, \( \omega \) is the field frequency, and \( \beta \) is the atom-cavity coupling constant; \( a \) and \( a\dagger \) are the bosonic lowering and raising operators, while \( \sigma^\pm \) are the atomic lowering and raising operators of the two level system. The eigenstate of this Hamiltonian are polaritons, or dressed states, given by a combination of atom and field states. In the base \( \{|0, \downarrow\rangle, |0, \uparrow\rangle, |1, \downarrow\rangle, |1, \uparrow\rangle, \ldots \} \), the atom states are represented in the basis of the eigenstates \( |\downarrow\rangle, |\uparrow\rangle \) of the Pauli \( \sigma_z \) operator, while the field states are denoted with the number operator’s eigenstates \( |n\rangle \). The Jaynes-Cummings Hamiltonian eigenstates are given by

\[
|n, -\rangle = \cos \theta_n |n, \downarrow\rangle - \sin \theta_n |n - 1, \uparrow\rangle \\
|n, +\rangle = \sin \theta_n |n, \downarrow\rangle + \cos \theta_n |n - 1, \uparrow\rangle 
\] (3.23)

for every \( n \geq 1 \), where the angle \( \theta_n \) is expressed in terms of the detuning parameter \( \Delta = \epsilon - \omega \) and is given by

\[ \theta_n = \frac{1}{2} \arctan \left( \frac{2\beta \sqrt{n}}{\Delta} \right). \] (3.24)

The eigenvalues associated to these eigenstates are given by

\[ E(n, \pm) = \omega n + \frac{\Delta}{2} \pm \sqrt{n\beta^2 \pm \frac{\Delta^2}{4}} \] (3.25)

In addition to the above dressed state, another eigenstate of the system is \( |0\rangle \equiv |0, \downarrow\rangle \), when \( n = 0 \), with the associated eigenvalue \( E_0 = 0 \). The fundamental state of the system should be determined for every fixed value of the parameters. Proceeding with this calculation we can observe first of all that the ground state will be either the state with zero polarizations \( |n = 0\rangle \) and energy \( E_0 = 0 \), or one of the states \( |n-\rangle \) associated to the eigenvalues \( E_{n,-} \). Indeed, for every fixed number of polaritons \( n \geq 1 \) we have \( E_{n,+} > E_{n,-} \). If we consider the
Figure 3.5: The energy non-linear dependence of the spectrum $E(n, \pm) - n\omega$ as a function of the detuning $\Delta$ for $\beta = 1$. The non-linearity effects are stronger for low values of $n$.

spectrum in the limit $\omega \gg |\Delta|$, $\beta$ the state with zero polaritons $|n = 0\rangle$ will be the ground state. As we decrease $\omega$ we will find a point in the parameter space where $E_0 = E_{1,-}$, precisely at $\omega = \Delta/2 - \sqrt{(\Delta/2)^2 + \beta^2}$. Lowering the value of $\omega$ further we will find a full set of degeneracy points given by (for $n \geq 1$)

$$\frac{\omega}{\beta} = \sqrt{n + 1 + \left(\frac{\Delta}{2\beta}\right)^2} - \sqrt{n + \left(\frac{\Delta}{2\beta}\right)^2}.$$  

(3.26)

The energy spectrum of the atom-cavity system, given by Eq. (3.25), has a nonlinear dependence on $n$ (see the energy spectrum in Figure 3.5). This anharmonicity in the splitting of the energy eigenstates gives rise to nonlinear phenomena at the single-photon level. One of the most relevant of these is photon blockade, where the presence of one photon stops further absorption of photons from a coherent light source [165–167].

### 3.3.3 Jaynes-Cummings-Hubbard model

Optical cavities containing trapped atoms can be arranged in arrays where the overlap between different cavities’ wave-functions allows photons to hop from one site to another. The Hamiltonian describing this new physical scenario is now known as Jaynes-Cummings-Hubbard model. The implementation of optical fibres, or other optical devices, can be
used to realize more complex geometries, where the hopping is not restricted to nearest neighbour cavities on a regular lattice [120–122]. This is precisely the kind of scenario we want to investigate in this part.

To tune the number of polaritons in each cavity a chemical potential $\mu$ might be used, hence the full JCH model will be described by the following Hamiltonian,

$$H^{JCH} = \sum_i \left[ H_i^{JC} - \mu N_i \right] + H^{hop}$$

(3.27)

where

$$H_i^{JC} = \epsilon \sigma_i^+ \sigma_i^- + \omega a_i^\dagger a_i + \beta (\sigma_i^+ a_i + \sigma_i^- a_i^\dagger)$$

(3.28)

is the Jaynes-Cummings Hamiltonian for a single cavity, and $N_i$ indicates the number of polaritons in each cavity ($N_i = \sigma_i^+ \sigma_i^- + a_i^\dagger a_i$); while $H^{hop}$ is the hopping term. Note that the chemical potential $\mu$ is not an experimentally tunable parameter for this system. In real experiments appropriate preparation schemes have to be devised in order to obtain states with different polariton number. Recently, using the Rabi model, it has been shown that the inclusion of counter rotating terms can stabilize finite-density quantum phases of correlated photons without the use of a chemical potential [155]. The last hopping term in Eq. (3.27) is characterized by $\kappa$ and the adjacency matrix of the underlying quantum network $\tau$, and is given by

$$H^{hop} = -\kappa \frac{1}{2} \sum_{i,j} \tau_{ij} (a_i^\dagger a_j + a_j^\dagger a_i).$$

(3.29)

We first consider two extreme cases: one in which the hopping strength is very small, and one where the atom-photon interaction is negligible. In the atomic limit $\kappa/\beta \ll 1$, the Hamiltonian $H^{JCH}$ becomes, to first order approximation, the sum of single cavity Hamiltonians $H = \sum_i H_i$, with $H_i$ given by

$$H_i = H_i^{JC} - \mu N_i.$$  

(3.30)

The eigenstates of the single cavity Hamiltonian are given by Eqs. (3.23) for $n \geq 1$, and
\[ |0, \downarrow \rangle = |0 \rangle \text{ for } n = 0. \] The corresponding eigenvalues are

\[
E_{n \pm}^\mu = (\omega - \mu)n + \frac{\Delta}{2} \pm \sqrt{n \beta^2 + \frac{\Delta^2}{4}},
\]

for \( n \geq 1 \), and \( E_0 = 0 \) for \( n = 0 \). The ground state of the system can be calculated similarly to the case of a single cavity. For every cavity we find that the ground state is constituted either by the eigenstate \( |n, -\rangle \) or by the eigenstate \( |0 \rangle \).

In the hopping dominated limit \( \kappa/\beta \gg 1 \) we can treat the atom-photon interaction perturbatively. \( H_{JCH} \) reduces, to first-order approximation, to a tight-binding hamiltonian \( H_{tb} \) given by

\[
H_{tb} = \sum_i (\omega - \mu)a_i^\dagger a_i - \frac{\kappa}{2} \sum_{i,j} \tau_{ij} (a_i^\dagger a_j + a_j^\dagger a_i).
\]

The eigenvalues of \( H_{tb} \) depends in a simple way from the eigenvalues \( \lambda_n \) of the adjacency matrix of the quantum network:

\[
E_n = N(\omega - \mu - \kappa \lambda_n).
\]

The above equation reveals an instability of the system for

\[
\kappa \Lambda > \omega - \mu
\]

where \( \Lambda \) is the maximal eigenvalue of the adjacency matrix \( \tau \). From this result it can be concluded that the maximal eigenvalue of the adjacency matrix sets an important scale for the strength of the hopping coefficient \( \kappa \).

3.3.3.1 Mean-field theory

To explore the phase diagram of the Jaynes-Cummings-Hubbard model, we make use of the mean-field treatment of the hopping term, which reduces to the following approximation

\[
a_i a_j^\dagger \simeq \langle a_i \rangle a_j^\dagger + a_i \langle a_j^\dagger \rangle - \langle a_i \rangle \langle a_j^\dagger \rangle.
\]
Therefore the hopping term becomes

\[
H_{\text{hop}}^{MF} = -\kappa \sum_{i,j} \tau_{ij}(a_i^\dagger + a_i)\psi_j + \kappa \sum_{i,j} \tau_{ij}\psi_i\psi_j,
\]  

(3.36)

where we have indicated by \(\psi_i\) the local order parameter \(\psi_i \equiv \langle a_i \rangle\) (also equal to \(\langle a_i^\dagger \rangle\), due to the gauge symmetry of the model). This Hamiltonian displays a phase transition between a Mott-Insulator phase, where \(\psi_i = 0\ \forall i\), and a superfluid phase. In order to study the phase diagram of this model, within the mean-field approximation we treat \(H_{\text{hop}}\) as a perturbation and we calculate \(\psi_i\) self-consistently, to first order in \(\kappa\), obtaining (see the Appendix for more details)

\[
\psi_i = \kappa \sum_j \tau_{ij}\psi_j R_n,
\]  

(3.37)

with \(R_n\) given by

\[
R_0 = \left[ \frac{\cos^2 \theta_1 + \sin^2 \theta_1}{E_{1-}^\mu} \right],
\]  

(3.38)

\[
R_{n \geq 1} = -\left[ \frac{\sqrt{n+1} \cos \theta_n \cos \theta_{n+1} + \sqrt{n} \sin \theta_n \sin \theta_{n+1}}{E_{n-}^\mu - E_{(n+1)-}^\mu} \right]^2
+ \frac{\sqrt{n+1} \cos \theta_n \sin \theta_{n+1} - \sqrt{n} \sin \theta_n \cos \theta_{n+1}}{E_{n-}^\mu - E_{(n+1)+}^\mu}^2
+ \frac{\sqrt{n} \cos \theta_n \sin \theta_{n-1} + \sqrt{n-1} \sin \theta_n \sin \theta_{n-1}}{E_{n-}^\mu - E_{(n-1)-}^\mu}^2
+ \frac{\sqrt{n} \cos \theta_n \sin \theta_{n-1} - \sqrt{n-1} \sin \theta_n \cos \theta_{n-1}}{E_{n-}^\mu - E_{(n-1)+}^\mu}^2
\]

where the integer \(n \geq 0\) depends on the system’s parameters and is chosen minimizing the onsite energy \(E_{n-}^\mu\) given by Eq. (3.31). If we diagonalize Eq.(3.37), along with the eigenvalues of the adjacency matrix \(\tau\), we get that the critical line for the transition between the Mott-insulator phase and the superfluid phase is given by

\[
\kappa \Lambda R_n = 1,
\]  

(3.39)

where \(\Lambda\) is the maximal eigenvalue of the adjacency matrix \(\tau\). This clearly shows that the phase diagram of the model depends on the product \(\kappa \Lambda\). On regular graphs we have
\[ \psi_i = \psi \ \forall i, \text{ and } \Lambda = z, \text{ where } z \text{ is the connectivity of the lattice.} \]

On the other hand, for complex topologies, the maximal eigenvalue of the hopping matrix \( \Lambda \) can be significantly different from the average connectivity of the networks. In particular, for a large variety of networks the maximal eigenvalue of the adjacency matrix \( \Lambda \) diverges with the network size. This suggests that, in order to have a non-trivial phase diagram for the Jaynes-Cummings-Hubbard model, the hopping strength \( \kappa \) must scale as

\[ \kappa \propto \frac{1}{\Lambda}. \]  

In the following sections we will investigate different network topologies for the respective scaling, with the network size, of the maximal eigenvalue of the adjacency matrix [150,151]. We note here that at the mean-field level the phase boundary is given by Eq. (3.39).

Regarding the phase diagram on regular lattices, the effect of the complex topology is the substitution of the average degree \( z \) of the lattice with the maximal eigenvalue \( \Lambda \) of the network. Therefore the dependence of the phase boundary on the detuning parameter \( \Delta \) is similar to the one observed in regular lattices [162]. In fact, as soon as the detuning is different from zero, the Mott lobes with mean polariton number greater than one are reduced in size and shifted to smaller value of the chemical potential. This effect is independent of the sign of the detuning parameter. We remark that on complex networks as in regular lattices the thermal fluctuations destroy the Mott insulator phase. Therefore at finite temperature the phase diagram should be composed of a superfluid regime and a normal fluid.

### 3.3.3.2 Regular networks

For regular networks and regular lattices with connectivity \( z \), the maximal eigenvalue of the adjacency matrix \( \Lambda \) is independent on the network size. In particular, we have

\[ \Lambda = z. \]  

In this case the critical line Eq. (3.39) coincides with the one found in the literature using the mean-field approximation [157–159].
Figure 3.6: Mean-field phase diagram of the Jaynes-Cummings-Hubbard model with $\Delta = 0$ on a random scale-free network with power-law exponent $\gamma = 2.2$ for different value of $N$, i.e. $N = 100$ (top panel) $N = 1000$ (middle panel) $N = 10000$ (bottom panel). The phase diagram scales with the maximal eigenvalue that is given by $\Lambda = 5.98$ (top panel) $\Lambda = 11.07$ (middle panel) and by $\Lambda = 23.42$ (bottom panel). The solid lines denote the analytic perturbative solution in mean field of the model.
3.3.3.3 Random graphs

For random Erdős-Renyi graphs with finite connectivity and Poisson degree distribution, it has been proven [151] that

$$\Lambda \propto \sqrt{k_{\text{max}}}, \quad (3.42)$$

where $k_{\text{max}}$ is the maximal degree of the system. For random networks with a finite connectivity we have $k_{\text{max}} = \ln N / \ln \ln N$, therefore

$$\Lambda(N) \propto \sqrt{\frac{\ln N}{\ln \ln N}}. \quad (3.43)$$

Considering the scaling given by Eq. (3.40), we have that the hopping strength has to satisfy the following relation in order to have a non-trivial phase diagram

$$\kappa(N) \propto \sqrt{\frac{\ln \ln N}{\ln N}}. \quad (3.44)$$

3.3.3.4 Random scale-free networks

Scale-free networks provide one of the most interesting and most studied topologies for the analysis of phase transitions occurring on them. Classically, the phase diagram of the Ising model [96–98, 109], and the percolation transition [100, 101] change drastically due to the diverging second moment of the average degree $\langle k^2 \rangle$ on scale-free networks with degree distribution $P(k) \propto k^{-\gamma}$ and power-law exponent $\gamma \in (2, 3]$. A similar observation can be made for the epidemic spreading model on annealed complex networks [102], i.e. complex networks in which the links are dynamically rewired. Moreover, the spectral properties of the complex networks determine the critical behavior of the epidemic spreading process on complex quenched networks [103, 104] for the $O(N)$ model [107, 108] and the stability of the synchronization dynamics [105, 106].

In random scale-free networks with power-law degree distribution $P(k) \propto k^{-\gamma}$, it has been proven [150] that the maximal eigenvalue scales like

$$\Lambda \propto \begin{cases} \sqrt{k_{\text{max}}} & \text{for } \gamma > 2.5 \\ \frac{\sqrt{\langle k^2 \rangle}}{\langle k \rangle} & \text{for } \gamma < 2.5. \end{cases}$$

The maximal degree of the network satisfies $k_{\text{max}} = \min \left[ N^{1/2}, N^{1/(\gamma-1)} \right]$, where we have considered the structural cutoff of the degrees of the network for $\lambda \leq 3$. Therefore, the
maximal eigenvalue of the network $\Lambda$ follows a different scaling with the network size, depending on the power-law exponent $\gamma$,

$$\Lambda(N) \propto \begin{cases} 
N^{1/[2(\gamma-1)]} & \text{for } \gamma > 3 \\
N^{1/4} & \text{for } 2.5 < \gamma \leq 3 \\
N^{(3-\gamma)/2} & \text{for } \gamma < 2.5.
\end{cases}$$

The hopping coefficient $\kappa$ that ensures a non-trivial phase diagram [see Eq. (3.40)] scales with the network size $N$ according to the following rules

$$\kappa(N) \propto \begin{cases} 
N^{-1/[2(\gamma-1)]} & \text{for } \gamma > 3 \\
N^{-1/4} & \text{for } 2.5 < \gamma \leq 3 \\
N^{-(3-\gamma)/2} & \text{for } \gamma < 2.5.
\end{cases}$$

Figure 3.6 shows both the analytic perturbative solution in mean-field of the JCH model, and the numerical non-perturbative mean-field evaluation of the phase diagram. As the figures show, there is substantial agreement between the two, and furthermore one can observe the dependence on the network size by the change in the critical lines.

### 3.3.3.5 Apollonian networks

In this section we consider Apollonian networks [113] which are constructed through a 2D Apollonian packing model in which the space between three tangent circles placed on the vertices of an equilateral triangle is filled by a maximal circle. The space-filling
procedure is repeated for every space bounded by three of the previously drawn tangent circles. The corresponding Apollonian network is constructed by connecting the centers of all the touching circles [Figure 3.7 (left)]. The resulting network is scale-free with power-law degree distribution $p(k) = Nk^{-\lambda}$ and $\lambda = 1 + \ln(3)/\ln(2) \simeq 2.585$. These networks are also known to have diverging maximal eigenvalue $\Lambda$ of their adjacency matrix [114]. In Figure 3.8 we plot the maximal eigenvalue $\Lambda$ of the apollonian network as a function of the network size $N$. We can fit the numerical results with the function

$$\Lambda(N) \propto N^{0.23}.$$  

(3.45)

Therefore the hopping coefficient $\kappa$ [that needs to scale according Eq. (3.40)] scales for large $N$ as

$$\kappa(N) \propto N^{-0.23}.$$  

(3.46)

Figure 3.8: Scaling of the maximal eigenvalue $\Lambda$ of the Apollonian network as a function of the size $N$ of the network.
Figure 3.9: The maximal eigenvalue of the Small-World network as a function of $p$ for different network sizes $N$. In the limit $p \to 0$ the small world model is a regular chain with average connectivity $z = 4$, therefore in this limit $\Lambda = 4$. The data are averaged over 100 network realizations.

3.3.3.6 Small-world networks

Networks combining the characteristics of random networks (a small diameter) and regular networks (a high clustering coefficient) are called small-world networks. [18]. Following the construction proposed in [18], we start from a regular chain in which each node is linked to the nearest neighbours and to the next-nearest neighbours and then rewire every link with probability $p$ to another random node of the network. For $p = 0$ the small-world network is a regular lattice in one dimension; for $p = 1$ the small-world network becomes one instance of a random network. For every intermediate value of $p$ we observe the small-world network with a small average diameter and a high clustering coefficient. The maximal eigenvalue of this network, for $p = 1$ will increase with $N$, as in the random graph case [Eq.(3.43)], while for the case of $p = 0$ it will be independent of $N$, as in regular networks. In Figure 3.9 we see how the maximal eigenvalue of a small-world network changes with $N$ for intermediate values of the probability $p$. 
3.3.4 Concluding Remarks

In this section, we have studied the Jaynes-Cummings-Hubbard (JCH) model on complex quantum networks. We demonstrated that the phase diagram derived in the mean-field approximation depends crucially on the maximal eigenvalue $\Lambda$ of the hopping matrix. In particular the phase diagram depends on the product $\kappa \Lambda$. This implies that in order to have a well defined phase diagram in the large network limit, the hopping coefficient $\kappa$ should scale proportional to $1/\Lambda$. For regular networks and lattices, the eigenvalue $\Lambda$ is equal to the connectivity of the network whereas for complex random networks it generally increases with the network size. We have also listed the scaling of the maximal eigenvalue $\Lambda$ with the network size $N$ for a large class of networks. For complex networks that have a diverging $\Lambda$, the hopping coefficient should be a decreasing function of $N$ in order to observe the phase transition from the Mott-like regime to the superfluid phase. This result implies the possibility of observing quantum critical behavior in arrays whose cavities are weakly coupled, assuming the effective realization of the proper complex quantum network topology.
Chapter 4

Dynamical Processes on Interacting and Multiplex Networks

A realistic description of many complex systems can be achieved by considering multiple layers of interacting networks. A non-trivial, multilayered connectivity has profound consequences on the dynamical processes taking place on these networks. Recent years have seen witnessed a high level of activity in the research on multilayer versions of dynamical processes on networks, most of which have completely novel characteristics. In this chapter of the thesis, we touch on two dynamical processes on interacting and multiplex networks, adding to the growing literature on the subject. In the first section, we propose a model of opinion dynamics on antagonistically interacting social networks and simulate the campaign process preceding an election. In the second part, we utilize the dynamics of the random walk process in the assessment of centrality on multiplex social network datasets and study the ranking with respect to this centrality.

4.1 Background

Most real-world systems are comprised of parts that interact with each other on multiple levels. This interaction can be in the form of interdependencies of different subsystems on each other, perhaps best exemplified by infrastructure systems. Alternatively, it could signify multiple types of interactions between the constituents of the system, which can be represented in different layers – a hallmark of social systems. Put in terms of complex
networks, the function of a node in one network can depend on the operational level of the nodes it is dependent on in other networks, or there might exist links of different types (colors) between the nodes of a network. For instance, the same individuals, groups and organizations can play different roles within a social relationship or can be linked through different types of social relationships (e.g., family relationships, acquaintanceship, friendship, and professional collaboration) [168–172], can have different affiliations [173, 174], and can communicate with one another using different technologies, such as mobile phone, chat, e-mail, or video conferences [175,176]. Each of these roles, relationships, affiliations, and communication technologies can in turn be associated with a different social network in which links between nodes refer to a distinct form of social interaction between the connected nodes. The same people, groups or organizations that interact in many different ways can thus be represented as the nodes of multiple co-evolving social networks that are themselves connected with one another as the various forms of social interaction affect one another over time [177–180].

In this more generalized and realistic framework of interacting and multilayered networks, many dynamical phenomena were found to be fundamentally different from those in the traditional single network approach. Buldyrev et al. demonstrated [181] on interdependent infrastructure networks an increased vulnerability due to cascading failures, contrary to what is expected from single complex networks. This and other initial studies on interdependent networks [181–185] paved the way for further interest in interacting networks. Investigated examples range from infrastructure networks as the power-grid and the Internet [181] to interacting biological networks in physiology [186].

The research on interacting networks has subsequently led to a greater interest in multiplex networks [186–190]. A system in which the same set of nodes belongs to multiple interacting and co-evolving networks is typically referred to as a multiplex network or multigraph [191,192]. In recent literature, there has been an upsurge of interest in multiplex networks. In particular, scholars have concentrated on the structural properties [180,193–196] and the antecedents [197,198] of these networks. Different models for capturing the structure of multiplexes have been proposed, including multiplex ensembles [199], growing multiplex models [200,201] and models based on tensor formalism [202].

Moreover, in order to have a better understanding of the dynamical evolution of interacting networks, many dynamical processes have been generalized in the framework of
multiple layered interacting networks. Of particular interest to this chapter, researchers have begun to shed light on dynamical processes such as diffusion processes [188,203], cooperation [190,204], exchange relations [205,206], percolation phase transitions [181,207], cascades [208] and epidemic spreading [209] occurring on them, and have developed modeling frameworks [199, 200, 210] and game-theoretic perspectives [190].

4.2 Opinion Dynamics in Antagonistically Interacting Social Networks

Relatively less explored until recently in the context of interacting networks is the case of interacting social networks, describing individuals that maintain their personal relationships in different social settings (e.g., work, family, friendship, etc.). Considering these multiple layers is crucial, as proven recently for community detection methods in social networks [211–213], but the effect of their presence is still not understood in many respects. For example, there is considerable current interest in opinion models [214], among which we cite the the Sznajd model [215], the voter model [216], the naming game [217,218] and Galam models [219,220]. However, the influence of more than one network has attracted less attention [221].

The model we propose in this section describes the opinion dynamics of two parties competing for votes during a political campaign. Each opinion, i.e., party, is modeled as a social network on which contagion dynamics can take place. An individual is represented by a node on each network, and can be active only in one of the two networks (vote for one party) at the moment of the election. Each agent has also a third option [217,218,222–224], namely not to vote, which translates into being inactive in both networks. Crucial to the model is the fact that agents are affected by the opinion of their neighbors meaning that the nodes tend to be active in the networks where their neighbors are also active. Furthermore, the chance of changing opinions decreases as the decision moment approaches, in line with the observation that vote preferences stabilize as the election day comes closer [225].

Here, we seek to gain insight into the role of multiple interacting social networks in the voting scenario through a simple and clear mathematical model, along the lines of, for example, recent work concerning the issue of ideological conflict [224]. We describe the dynamics of social influence in the two networks, and we model the mitigation of uncertainty prior to the vote through a simulated annealing process. Long before the election,
the agents change opinions and can sustain a small fraction of antagonistic relations, but as the election approaches their dynamics slows down, until finally they reach the state in which the dynamics is frozen, at the election day. At that moment, the winning party is the one with more active nodes. Given this framework, we focus on the case where the networks sustaining each party are represented by two Poisson random graphs, and address the role of different average connectivities. This choice of degree distribution is consistent, as an example, with the data on social networks of mobile phone communication, which are characterized by a typical scale in the degree (being fitted with a power-law distribution of exponent $\gamma = 8.4$) [226].

4.2.1 The election model: Parties as antagonistic social networks

The model describes two antagonistic networks $A, B$ representing the social networks of two competing political parties. Each agent $i$ is represented in both networks and can choose to be active in either one of the networks. We define the activity such that $\sigma^A_i = 0$ if agent $i$ is inactive in network $A$ and $\sigma^A_i = 1$ if agent $i$ is active in network $A$. Similarly $\sigma^B_i = 0, 1$ indicates if a node is inactive or active in network $B$. Since the activity of an individual in a network ultimately corresponds to the agent voting for the corresponding party, each agent can be active on only one network on the election day (i.e. if $\sigma^A_i = 1$ then $\sigma^B_i = 0$ and if $\sigma^B_i = 1$ then $\sigma^A_i = 0$). Nevertheless the model gives the agent the freedom not to vote, in which case $\sigma^A_i = \sigma^B_i = 0$. Moreover agents are influenced by their neighbors. To account for this influence, we assume that on the election day, if at least one neighbor of agent $i$ is active in network $A$, the agent will be active in the same network (network $A$) provided that it is not already active in network $B$. We assume that a symmetrical process is occurring for the opinion dynamics in network $B$. Therefore, the mathematical constraints that our agent opinions need to satisfy at the election day are:

\[
\begin{align*}
\sigma^A_i &= \left[ 1 - \prod_{j \in N_A(i)} (1 - \sigma^A_j) \right] (1 - \sigma^B_i) \\
\sigma^B_i &= \left[ 1 - \prod_{j \in N_B(i)} (1 - \sigma^B_j) \right] (1 - \sigma^A_i),
\end{align*}
\]

where $N_A(i)$ ($N_B(i)$) are the set of neighbors of node $i$ in network $A$ (network $B$). On the election day, people cannot change their opinion anymore. On the other hand, before the election day we allow for some conflicts in the system, and in general the constraints
provided by Eqs. 4.1 will not be satisfied.

4.2.2 Evolution dynamics during the election campaign

In order to model the decision process of agents on their vote during the pre-election period, we consider the following algorithm. We propose a Hamiltonian that counts the number of the constraints in Eq. (4.1) that are violated. We take a Hamiltonian $H$ of the following form

$$
H = \sum_i \left\{ \sigma_i^A - \left[ 1 - \prod_{j \in N_A(i)} (1 - \sigma_j^A) \right] (1 - \sigma_i^B) \right\}^2 + \\
\sum_i \left\{ \sigma_i^B - \left[ 1 - \prod_{j \in N_B(i)} (1 - \sigma_j^B) \right] (1 - \sigma_i^A) \right\}^2.
$$

(4.2)

Since the terms in the brackets can take on the values $\pm 1, 0$, a natural choice of Hamiltonian to count the number of constraint violations involves squares of these terms.

The dynamics starts from an initial condition where the active nodes in networks A and B are distributed uniformly randomly, and we consider the fact that long before the election, the agents are free to change opinions. Formally, we model their dynamics as a Monte Carlo dynamics which equilibrates following the Hamiltonian $H$ starting from a relatively high initial temperature, i.e. initially some conflicts are allowed in the system. Therefore the active nodes in networks A and B are initially distributed according to the high temperature Gibbs measure, mimicking an effectively “unbiased” population at the beginning of the campaigning process. Moreover, since we start with a sufficiently high temperature, the dynamics does not depend on the specific initial conditions of the system. As the election day draws near, the effective temperature of the opinion dynamics decreases and the agents tend to reduce the number of conflicts with their neighbors to zero.

The opinion dynamics described above is implemented with a simulated annealing algorithm. We start at a temperature $T = 1$ and we allow the system to equilibrate by $2N$ Monte Carlo steps where a node is picked randomly in either one of the networks with equal probability and is changed from active to inactive or vice versa. Subsequently, the Hamiltonian, or the number of conflicts, is recalculated. If the opinion flip results
Figure 4.1: The two competing political parties are represented by two networks. Each agent is represented in both networks but can either be active (green node) in only one of the two, or inactive (red node) in both networks. Moreover the activity of neighbor nodes influence the opinion of any given node.
in a smaller number of conflicts, it is accepted. Otherwise, it is accepted with probability $e^{-\Delta H/kT}$. This Monte Carlo process is repeated by slowly reducing the temperature by a multiplicative factor of 0.95 until we reach the temperature state $T = 0.01$ where the Hamiltonian is $H = 0$ meaning there are no more conflicts in the network, and the probability of one opinion flip is about $e^{-1/0.01} \approx 10^{-44}$. The choice of increment in the temperature reduction is such that the overall simulation time is compatible with the dynamics of social systems. The Monte Carlo sweeps that are performed, each of which corresponds to one campaigning day, span a total number of $\log 0.01/\log 0.95 \approx 90$ days. It turns out that the Hamiltonian $H$ has in general multiple fundamental states and the simulated annealing algorithm always find one of these states. An example of the final configuration for the model just described is depicted in Figure 4.1.

4.2.3 The phase diagram for two Poissonian networks

Here we report the result of this opinion dynamics for two antagonistic networks $A, B$ with Poisson degree distributions and different average connectivities $z_A, z_B$, respectively. We plot the size $S_A$ of the giant component of the percolating cluster in network $A$, i.e. the largest connected component of active nodes in network $A$, as a function of the average connectivities (Figure 4.2). We observe a rich phase diagram of the opinion dynamics, consistent with the following scenario valid in the limit of large network sizes:

- **Region (I) in Figure 4.2:** $z_A < 1, z_B < 1$. In this region both giant components in network $A$ ($S_A$) and network $B$ ($S_B$) are zero, $S_A = 0, S_B = 0$, and therefore essentially agents never vote.

- **Region (II) in Figure 4.2:** In this region the giant component in network $B$ emerges, $S_B > 0, S_A = 0$.

- **Region (III) in Figure 4.2:** In this region the giant component in network $A$ emerges, $S_A > 0, S_B = 0$.

- **Region (IV) in Figure 4.2** In this region we have the pluralism solution of the opinion dynamics and giant components in both network $A$ and network $B$ are different from zero, $S_A > 0, S_B > 0$.

In Regions II (III) the active agents in party $B$ (party $A$) percolate the system while agents in party $A$ (party $B$) remain in disconnected clusters. On the other hand, in the
Figure 4.2: (Panel A) The size of the largest connected component $S_A$ in network A at the end of the simulated annealing calculation as a function of the average connectivity of the two networks: $z_A$ and $z_B$ respectively. The data is simulated for two networks for $N = 500$ nodes and averaged 60 times. The simulated annealing algorithm is independent of initial conditions. The white line represents the boundary between the region in which network A is percolating and the region in which network A is not percolating. (Panel B) The schematic representation of the different phases of the proposed model. In region I none of the networks is percolating, in region II network B is percolating in region III network A is percolating in region IV both networks are percolating.
Figure 4.3: We represent the fraction of nodes in the giant component $S_A$ of network A and in the giant component $S_B$ of network B in different regions of the phase space. In region II ($z_A = 1.5, z_B = 4$) the giant component in network A ($S_A$) disappears in the thermodynamic limit while in region IV ($z_A = 2.5, z_B = 4$) it remains constant. The giant component in network B remains constant in the thermodynamic limit both in region II and region IV. Each data point is simulated for the two networks for $N$ nodes and averaged 200 times.

case where the average connectivity of the two parties is comparable (Region IV), the system can sustain an effective pluralism of opinions with both parties percolating in the system. To reiterate, we reach the finding that if the connectivity of both parties is large enough, i.e. we are in region IV of the phase diagram (Figure 4.2B), pluralism can be preserved in the model and there will be two parties with a high number of votes. As part of our study, we also characterize the finite size effects. We show in Figure 4.3 that in region II ($z_A = 1.5, z_B = 4$) the giant component in network A ($S_A$) disappears in the thermodynamic limit while in region IV ($z_A = 2.5, z_B = 4$) it remains constant.

For a party to win the election, it is necessary that the active agents percolate in the corresponding network. Still, the election outcome depends crucially on the total number of votes in network A ($m_A$) and the total number of votes in network B ($m_B$). In Figure 4.4 we plot the difference between the number of votes in network A and the number of votes in network B, i.e. $m_A - m_B$. We observe that the more connected party (network) has the majority of the votes. It is also worth noting that the final outcome of the election is not affected by the initial conditions. Overall, this result supports the intuition that the party with the more connected supporting network will win the elections, and is in
The role of committed agents [218, 224, 228] have recently been considered in different opinion-dynamics models. In this section we explore the effect of committed individuals during the election campaign by considering the case where a fraction of the nodes always remain active in one of the two networks, never changing their opinion. Figure 4.5 shows that in Region IV, where the average connectivity of the two parties are similar and small perturbations could alter the results, a small fraction of agents $f \simeq 0.1$ in the less connected network can reverse the outcome of the election. Indeed the probability distribution $P = P(m_B - m_A)$ of different realizations of the dynamics is shifted towards the party agreement with recent results concerning the persuasive role of densely connected social networks on the adoption of a behavior [227].

4.2.4 Committed agents

The role of committed agents [218, 224, 228] have recently been considered in different opinion-dynamics models. In this section we explore the effect of committed individuals during the election campaign by considering the case where a fraction of the nodes always remain active in one of the two networks, never changing their opinion. Figure 4.5 shows that in Region IV, where the average connectivity of the two parties are similar and small perturbations could alter the results, a small fraction of agents $f \simeq 0.1$ in the less connected network can reverse the outcome of the election. Indeed the probability distribution $P = P(m_B - m_A)$ of different realizations of the dynamics is shifted towards the party...
supported by the committed minority. Remarkably, this finding fits perfectly with the results of the radically different models proposed in [218, 224], and generalizes them to the case of political elections. With this addition to the literature, the important role potentially played by committed minorities is thus suggested by several different models in different aspects of social dynamics, suggesting the need for future work exploring these findings.

4.2.5 Concluding Remarks

To conclude this section, we have proposed a simple model for the opinion dynamics taking place during an election campaign. We have modeled parties (or opinions) as antagonistic social networks, and individuals as nodes belonging to these social networks and connecting them. We have considered the case where individuals either have to decide on a single party, or neither of them. We have described the quenching of opinions preceding the voting moment as a simulated annealing process where the temperature is progressively lowered until the voting moment, at which point the individuals minimize the number of conflicts with their neighbors. We have demonstrated that there is a wide region in the phase diagram where both parties survive collecting a finite fraction of the votes, and hence the existence of pluralism in the election system. Furthermore, we have pointed out that a key quantity to get a finite share of the overall number of votes is the connectivity of the networks corresponding to different parties. That being said, connectivity is not sufficient to win the elections as a small fraction of committed agents is sufficient to invert the results of the voting process.

Being a basic model on purpose, our model provides insights into different aspects of the election dynamics. It can be interpreted as a model of any opinion formation process involving different contexts/networks, where opinions are frozen at some point in time, and where the agents’ behavior reflects the approaching of that point such that they are initially less susceptible to influence from their neighbourhoods (high initial temperatures) and attempt to reduce the level of frustration/conflict more strongly later (low temperatures). Future works could focus on generalizing the model by studying antagonistic networks with different topologies, such as competing scale-free and Poisson networks or two competing scale-free networks. Other extensions of this model could describe several competing parties, consider a threshold dynamics like the one triggering the opinion formation of the agents in [227], or relax the hypothesis of purely antagonistic interactions, thus allowing the agents to express multiple preferences in a multi-layered opinion space.
Figure 4.5: We represent the role of a fraction $f$ of committed agents in reverting the outcome of the election. In particular we plot the histogram of the difference between the fraction of agents $m_B/N$ voting for party $B$ and the fraction of agents $m_A/N$ voting for party $A$ for a fraction $f_A$ of committed agents to party $A$, with $f_A = 0$ and $f_A = 0.1$ and average connectivities of the networks $z_A = 2.5, z_B = 4$. The histogram is performed for 1000 realizations of two networks of size $N = 1000$. In the inset we show the average number of agents in network $A$ ($m_A$) and agents in network $B$ ($m_B$) as a function of the fraction of committed agents $f_A$. A small fraction of agents ($f_A \simeq 0.1$) is sufficient to reverse the outcome of the elections. The data in the inset is simulated for two networks for $N = 1000$ nodes and averaged 10 times.
4.3 Dynamics of Centrality Ranking in Multiplex Networks

Among the structural properties of multiplex networks that scholars have only recently begun to address [229, 230], a crucial role is played by the centrality of nodes. In a multiplex network, the importance of a node depends on the connectivity patterns within and across the different layers of the network. For univariate networks in which no more than one link can connect the same pairs of nodes, a number of measures are available for assessing the importance of nodes. Over recent years these measures have become increasingly popular and salient for a variety of empirical domains. Among these measures, in this thesis we concentrate our attention on PageRank, a centrality measure that has been successfully used not only for ranking web pages [231], but also for ranking scientists in citation networks [232] or species in food webs [233]. While PageRank was originally proposed as a centrality measure for univariate networks [231], its extension to multiplex networks remains largely unexplored. Compared to univariate networks, multiplex networks enable nodes to be connected with one another through multiple links co-evolving in multiple layers, thereby offering a richer and more detailed backdrop against which the structural position of nodes can be assessed. The ranking of nodes in one layer can affect, and be affected by, the ranking of the same nodes in other layers. A ranking of nodes can thus be obtained that is likely to differ from the one originating simply from the position of nodes in one single network. The extension of PageRank to multiplex networks is therefore expected to shed light on novel ways for measuring the importance of nodes that capture their embeddedness in multiple interrelated ways. This section attempts to address this non-trivial problem by proposing a generalization of PageRank to the case of multiplex networks.

4.3.1 PageRank

Introduced as a centrality measure to evaluate the relative “importance” of web pages, PageRank centrality draws on the idea of a web surfer that visits different parts of the WWW at random. The random walker follows two strategies: the first is to jump to a node selected uniformly at random; the second is to jump, still randomly, to one of the walker’s neighbors. The popularity of a node is a function of the frequency with which the random walker visits the node. This frequency is then compared with the frequencies associated with all other nodes in the network. The ranking of nodes obtained according to these frequencies of being visited is precisely the ordering produced by the PageRank
centrality measure, and reflects the relative popularity that each node has across the whole network.

The PageRank $x_i$ of a node $i$ in a network with $N$ nodes is defined as [231]

$$ x_i = \alpha A \sum_j A_{ij} \frac{x_j}{g_j} + (1 - \alpha_A) \frac{1}{N}, $$

(4.3)

where $A_{ij}$ are the elements of the adjacency matrix that are equal to one if node $j$ points to node $i$ and zero otherwise, $g_j = \max(1, k_{j_{\text{out}}}) = \max(1, \sum_r A_{rj})$, and $\alpha_A > 0$ is called the damping factor. PageRank can be interpreted as the stationary distribution of a random walk with additional random jumps. A random walker on site $j$ jumps to one of $j$’s $k_{j_{\text{out}}}$ out-neighbors with probability $\alpha_A$, and to any other site chosen uniformly at random with probability $1 - \alpha_A$. The PageRank of a node is large to the extent that many other nodes point to it. The PageRank of a node is therefore expected to increase as a function of the node’s in-degree, and indeed in [234, 235] it was shown that, for uncorrelated networks, the PageRank of nodes can be approximated by their in-degree. If nodes in uncorrelated networks are grouped into classes depending on their extended degrees $k = (k_{\text{in}}, k_{\text{out}})$, then the average PageRank for nodes of degree-class $k$ is

$$ \bar{x}(k) = \alpha A \frac{k_{\text{in}}}{\langle k_{\text{in}} \rangle N} + (1 - \alpha_A) \frac{1}{N}, $$

(4.4)

where the symbol $\langle \ldots \rangle$ indicates the average over the $N$ nodes of the network.

PageRank was originally proposed for ranking web pages in response to text queries, and for this reason it was formalized as a centrality measure for directed networks [231]. It is, however, possible to extend the original definition to the case of undirected networks. For these networks, PageRank is

$$ x_i = \alpha A \sum_j A_{ij} \frac{x_j}{g_j} + (1 - \alpha_A) \frac{1}{N}, $$

(4.5)

where $g_j = \max(1, k_j)$ and $k_j$ is the degree of node $j$. For undirected networks, the average PageRank $\bar{x}(k)$ of a node with degree $k$ is given by

$$ \bar{x}(k) = \alpha A \frac{k}{\langle k \rangle N} + (1 - \alpha_A) \frac{1}{N}. $$

(4.6)
4.3.2 Multiplex PageRank

In this part, we offer a generalization and extension of the PageRank measure that can be applied to any multiplex network dataset. The assumption underlying our proposed measure is that the centrality of a node in one network can be affected by the centrality of the same node in another network. For the sake of simplicity, we consider the case in which the multiplex network is organized into two layers: network A and network B. Our analysis can easily be generalized to multiplex networks with more than two layers (See Appendix A.3). We indicate with $A_{ij}$ the elements of the adjacency matrix of network A, and with $B_{ij}$ the elements of the adjacency matrix of network B. For network A, we evaluate PageRank $x = \{x_1, \ldots, x_N\}$ using Eq. (4.3) with the parameter $\alpha_A > 0$. We then express the Multiplex PageRank centrality $X = \{X_1, \ldots, X_N\}$ of the nodes in network B with respect to PageRank $x$.

Formally, we define the Multiplex PageRank centrality $X_i$ of node $i$ as

$$X_i = \alpha_B \sum_j x_i^j B_{ij} \frac{X_j}{G_j} + (1 - \alpha_B) \frac{x_i^j}{N(x^j)}, \quad (4.7)$$

where $G_j = \sum_r B_{rj} x_r^\gamma + \delta(0, \sum_r B_{rj} x_r^\beta)$, $\delta(a, b)$ is the Kronecker delta, $\alpha_B > 0$ is small enough to guarantee that the relation can be satisfied, and the exponents $\beta$ and $\gamma$ are both greater than or equal to zero. The first term in Eq. (4.7) refers to the contribution to node $i$’s centrality that derives from the centrality of the nodes pointing to $i$ in network B. Like with the ordinary PageRank measure, this contribution is inversely proportional to the out-degree of node $i$’s in-neighbors. However, unlike the ordinary measure, Eq. (4.7) enables this contribution to be also affected by the centrality that both node $i$ and its in-neighbors in network B have in network A. This interplay between the two networks has a two-fold effect on a node’s centrality. First, the extent to which node $i$ can derive some advantage from the centrality of its in-neighbors in network B becomes more significant as the centrality of $i$ in network A becomes larger. The more prominent a node is in one layer, the more likely it is that the node can attract and gain benefit from other important nodes in another layer. Second, the contribution of each in-neighbor $j$ to $i$’s centrality in network B is discounted by dividing $j$’s centrality by the sum of the centralities that $j$’s out-neighbors in network B have in network A. In other words, the benefits node $i$ can derive from the centrality of any in-neighbor $j$ in network B are diluted to the extent that $j$ in network B points to many other nodes that are associated with high centrality.
in network A. An important node in one layer can attract important nodes in a different layer, but the benefit that can be gained in so doing are mitigated if there are many other nodes that have a similar capacity of attraction.

The second term in Eq. (4.7) reflects the contribution to node $i$’s centrality in network B that derives from $i$’s centrality in network A. By adding this second term, nodes that are not able to attract important neighbors in network B, can still derive some advantage simply by being central in network A. In the extreme case, a node with a zero in-degree in network B can still be associated with a non-zero value of centrality if the node has a non-zero centrality in network A. The assumption underlying this component of centrality is that the importance of a node in one layer is positively affected by the importance that the same node has in another layer, regardless of the node’s capacity to attract other important nodes in the former layer.

Alternatively, Multiplex PageRank can also be regarded as the stationary distribution of a random walk with additional biased jumps. With probability $\alpha_B$, a random walker on site $j$ jumps to site $i$, one of $j$’s $k^\text{out}_j$ out-neighbors selected with probability proportional to $x^\beta_i$, and with probability $1 - \alpha_B$ jumps to site $i$ chosen with probability proportional to $x^\gamma_i$.

In what follows, we identify four important limiting cases of the Multiplex PageRank measure:

- **Additive Multiplex PageRank ($\beta = 0, \gamma = 1$):**

\[
X_i = \alpha_B \sum_j B_{ij} \frac{X_j}{G_j} + (1 - \alpha_B) \frac{x_i}{N(x)},
\]

(4.8)

where $G_j = \max(1, \sum_r B_{rj})$. This refers to the case in which the effect of network A on network B is exerted simply by “adding” some value to the centrality the nodes have in network B in proportion to the centrality they have in network A. Here the interplay between networks does not imply that the importance a node has in one network affects the node’s ability to derive benefits from important nodes in another network. Simply, being central in network A enables a node to gain more centrality in network B, regardless of the node’s capacity to attract important others in network B. Recast in terms of a random walk, this version of Multiplex PageRank refers to the case of a biased random walk, where the bias lies in the random jump to any node in network B. In particular, nodes with high PageRank in network
A are preferred over other nodes with low PageRank in the same network as the destination of the random jumps that the walker makes in network B. A similar version of this PageRank measure, in which the random jumps are biased according to some predetermined distribution called “personalized vector”, has already been suggested in the computer science literature [236]. In qualitative agreement with this version, here we propose to regard a node’s PageRank in one layer as the node’s “personalized vector” in another layer.

- **Multiplicative Multiplex PageRank** ($\beta = 1$, $\gamma = 0$):

\[
X_i = \alpha_B \sum_j x_i B_{ij} \frac{X_j}{G_j} + (1 - \alpha_B) \frac{1}{N},
\]

where $G_j = \sum_r B_{rj} x_r + \delta(0, \sum_r B_{rj} x_r)$. This refers to the case in which the effect of network A on network B lies in “multiplying” the benefits that a node gains from the importance of its in-neighbors in network B by a factor that is proportional to the node’s importance in network A. Thus, all benefits that can be obtained by being central in network A are contingent upon the connections that a node receives from important nodes in network B. The more important a node is in network A, the more value the node can extract from the connections received from important others in network B. Unlike the Additive version, the Multiplicative Multiplex PageRank does not enable a node to derive any added benefit in network B by simply being important in network A, regardless of the importance of the node’s in-neighbors in network B. Alternatively, this version of the measure also refers to the case of a biased random walk, where the bias lies in the walker’s choice of the out–neighbor as the destination of the jump. In particular, neighbors with high PageRank in network A are preferred over other neighbors with low PageRank in the same network.

- **Combined Multiplex PageRank** ($\beta = \gamma = 1$):

\[
X_i = \alpha_B \sum_j x_i B_{ij} \frac{X_j}{N(x)} + (1 - \alpha_B) \frac{x_i}{\langle x \rangle},
\]

where $G_j = \sum_r B_{rj} x_r + \delta(0, \sum_r B_{rj} x_r)$. This refers to the case in which the effect of network A on network B lies in “combining” the additive and multiplicative benefits a node in network B can gain by being central in network A. In this case, a node’s high centrality in network A can boost its centrality in network B both in itself and at the same time by amplifying the node’s ability to derive centrality from other
important nodes. Alternatively, this version of Multiplex PageRank refers to the
case in which both the destination of the random jump and the selection of the
random walker’s out-neighbor in network B are biased in that they favor nodes with
high PageRank in network A over nodes with low PageRank in the same network.

• **Neutral Multiplex PageRank** ($\beta = \gamma = 0$):

$$X_i = \alpha_B \sum_j B_{ij} \frac{X_j}{G_j} + (1 - \alpha_B) \frac{1}{N},$$

where $G_j = \max(1, \sum_r B_{rj})$. This refers to the case in which there is no effect of
network A upon network B, and thus Multiplex PageRank reduces to the PageRank
based simply on network B in isolation.

Clearly these limiting cases can be generalized so as to be applied also to a multiplex
network that combines two undirected networks or a directed network and an undirected
one. Moreover, the above definitions can be further generalized so as to accommodate
cases in which the rankings $x$ are obtained using different centrality measures, such as the
eigenvector centrality.

### 4.3.3 Mean-Field Approximation and Numerical Results

Following [234,235], we performed a mean-field calculation of the average Multiplex PageRank
$\overline{X}(k_B, x)$ of a node with degree $k_B = (k_B^{in}, k_B^{out})$ in network B and PageRank $x$ in
network A. We define $\overline{X}(k_B, x)$ in the following way

$$\overline{X}(k_B, x) = \frac{1}{N P(k_B, x)} \sum_{i|k_{B,i} = k_B} X_i,$$

where $P(k_B, x)$ is the probability that a node has degree $k_B = (k_B^{in}, k_B^{out})$ in network B
and PageRank $x$ in network A. In particular, performing a mean-field calculation (see
Appendix A.2) valid for an uncorrelated network B, we obtain

$$\overline{X}(k_B, x) = \alpha_B x^\beta k_B^{in} \frac{1}{\langle x^\beta k_B^{in} \rangle N} + (1 - \alpha_B) \frac{x^\gamma}{N \langle x^\gamma \rangle}.$$  

To verify the validity of Multiplex PageRank, we generated a duplex network with $10^7$
nodes and $8 \times 10^7$ links in each layer. In both layers, the in- and out-degrees decay as
a power law $k^\eta$, where $\eta_A^{out} = 2.8$, $\eta_A^{in} = 2.1$ and $\eta_B^{out} = 2.5$, $\eta_B^{in} = 2.5$. The dependence
of the Additive, Multiplicative, and Combined versions of PageRank upon in-degree is shown in Fig. 4.6. For small values of PageRank, the deviation from the diagonal is due to large fluctuations of PageRank in correspondence of small values of in-degree, as was also observed by Fortunato et al. [234].

4.3.4 Application to a Multiplex Dataset of Online Communications

To clarify the meaning of the four versions of Multiplex PageRank, we apply these measures to a multiplex network formed by the juxtaposition of two networks, and show that the centrality of a node in one network depends on the centrality of the same node in the other network. Our application is concerned with online communication and is based on a multiplex network in which the same users can interact by sending instant messages to one another and by posting messages to a forum. As users can send messages directly to one another and at the same time participate in discussion groups within a forum, they can be regarded as embedded in two related online social networks. Our results show that the Multiplicative Multiplex PageRank of users displays a broad distribution, and is thus able to capture the emergence of high-ranked nodes, unlike what can be obtained through the application of the PageRank centrality measure to a single network.

We apply the Multiplex PageRank measure to the multiplex network created from an online community at the University of California, Irvine [237]. The multiplex network
includes two layers. The first layer corresponds to a directed instant messaging (IM) network in which a directed link is established from one user to another if the former sends one or more online instant messages to the latter. The second layer is a bipartite network in which a link is established between a user and a discussion group of a forum when the former posts a message to the latter. While the IM network dataset covers the period from April 19 to October 26, 2004, the forum became active at a later time when users were already communicating through instant messages. The bipartite network thus covers a more restricted period than the IM network, from May 14 to October 26, 2004. The two networks also differ in the number of users: the total number of active users recorded for the IM network is 1,899, of whom only 899 posted at least one message in the forum. Moreover, users that were active in the forum created 552 thematic groups, each aimed at the discussion of a specific topic.

The analysis of the multiplex network covers the restricted observation period beginning on June 4, 2004, when both networks were operational and exhibited a fairly stable pattern of activity. At any specific day, and with a daily frequency, we constructed the instantaneous cumulative networks reflecting all the social interactions that took place in the three weeks' period ending on that day. Measurements thus create a time series with 124 sample networks starting on June 25, 2004. The multiplex network can be represented by the juxtaposition of the two time-varying adjacency matrices $A(t)$ and $B(t)$ that describe the IM network and the one-mode projection of the bipartite forum network, respectively (see Fig. 4.7). In particular, the adjacency matrix $A(t)$ describes directed links between users, i.e. $A_{ij}(t) = 1$ if user $j$ sent at least one message to user $i$ in a given time window. For the forum network, the adjacency matrix $B(t)$ describes an undirected and unweighted network between the users of the forum, where $B_{ij}(t) = 1$ if both user $i$ and user $j$ posted at least one message to a common discussion group in a given time window.

The application of Multiplex PageRank to online communication is motivated by the fact that users can enhance their ranking by engaging in multiple and interrelated ways of communication. In our specific case, users’ prominence in the IM network (A) is likely to have an impact upon the prominence they gain by communicating and interacting in the forum network (B). To fully capture this intertwined nature of users’ prominence, we begin by calculating each user’s PageRank $x_i$ based on the IM network. The Multiplex PageRank $X_i$ of user $i$ in the forum is then obtained by expressing the PageRank user $i$ has in the forum as a function of the user’s PageRank $x_i$ based on the IM network.
Figure 4.7: Sketch of the multiplex online social network in which users communicate by exchanging instant messages and by posting messages to a forum.

Formally, the Multiplex PageRank of user $i$ in the forum at time $t$ is

$$
X_i(t) = \alpha_B \sum_j [x_i(t)]^\beta B_{ij}(t) \frac{X_j(t)}{G_j(t)} + (1 - \alpha_B) \frac{[x_i(t)]^\gamma}{\langle [x(t)]^\gamma \rangle_B N_F(t)},
$$

(4.14)

where $N_F(t)$ is the number of active users in the forum at time $t$, $\langle \ldots \rangle_B$ denotes the average of $x(t)$ based only on the nodes that belong to network $B$ at time $t$, and $G_j(t) = \sum_r B_{rj}(t)[x_r(t)]^\beta + \delta(0, \sum_r B_{rj}(t)[x_r(t)]^\beta)$. In the above formula, the PageRank $x_i$ of node $i$ in the IM network at time $t$ is given by

$$
x_i(t) = \alpha_B \sum_j A_{ij}(t) \frac{x_j(t)}{g_j(t)} + (1 - \alpha_B) \frac{1}{N},
$$

(4.15)

with $g_j(t) = \max(1, k_j^{A, \text{out}}(t))$. For the IM-forum multiplex network, we compared the values of Multiplex PageRank with the theoretical expectations obtained in the case of an uncorrelated network. We found a very good agreement between the two sets of values (see Fig. 4.8).

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Figure 4.8: The Additive, Multiplicative, Combined, and Neutral users’ Multiplex PageRanks $X$ plotted against the mean field expectation $X_{th}$ (solid line) for the IM-forum multiplex network dataset. The damping factors used for the IM and forum data are $\alpha_A = \alpha_B = 0.85$.

A crucial issue affecting a large number of applications, ranging from the online sale of books to usage of Twitter tags, that rely on measures for ranking items is concerned with the stability of the rankings over time [238]. To address this problem, here we investigate the stability of the top-ranked users in the forum, and compare the rankings obtained using the different proposed versions of Multiplex PageRank.

In order to evaluate the stability of rankings in our dataset, we select the top five users with the highest Multiplex PageRank at the end of the whole observation period ($t = 124$), and track their evolution over time. In Fig. 4.9 we plot the time evolution of the values of PageRank $X$ of the five users with the highest Additive, Multiplicative, Combined, and Neutral PageRanks. Users are ranked in decreasing order, from top to bottom.
figure indicates that the top five users with the highest values of Multiplicative Multiplex PageRank and Combined Multiplex PageRank are the same, and the top five users with the highest values of Additive and Neutral Multiplex PageRank are the same (with the exception of user 297 and user 511; note that user 297 has extremely high PageRank in the IM network). The Neutral Multiplex PageRank refers to the case in which $\beta = 0$ and $\gamma = 0$ in Eq. (4.7), and thus produces a ranking of users that coincides with the one obtained by taking into consideration only users’ position in the forum.

When the importance of the users in the forum is adjusted to also reflect their position in the IM network simply by adding a bias in the random jump to any node, as occurs with the Additive Multiplex PageRank, the identity of the top five users in the resulting ranking does not change significantly. On the contrary, the introduction of a bias in the random walker’s choice of the out-neighbor as the destination of the jump, as occurs with the Multiplicative Multiplex PageRank, is responsible for a substantial change in the ranking of users. In particular, the emergence of new top-ranked users when the Multiplicative Multiplex PageRank is adopted suggests that there are synergies between the activities of these users in the IM and forum networks. The way they communicate and rise to prominence in one network affects how they communicate and rise to prominence in the other network. Thus, taking into account the multiplex nature of the dataset helps unveil these synergies and the multi-faceted nature of users’ prominence that would otherwise remain undetected if only one layer were investigated. Moreover, Fig. 4.9 shows that the Combined Multiplex PageRank, by adding a bias both in the random jump to any node and in the walker’s choice of the out-neighbor, does not produce any substantial change in the ordering of the top-ranked users with respect to the ranking that is obtained with the Multiplicative Multiplex PageRank.

In most applications, the use of PageRank for assessing the importance of nodes is aimed primarily at producing a ranking of nodes rather than associate each of them with a specific value of centrality. As in a variety of networks nodes’ PageRank is closely related to their in-degree, especially for nodes with high in-degree, it has become common practice to use in-degree as a proxy for PageRank. In the case of the multiplex online social network, drawing on our theoretical framework, we tested the hypothesis that the Additive Multiplex PageRank correlates with a linear combination of nodes’ in-degree in network A and their degree in network B, while the Multiplicative PageRank correlates with the product between nodes’ in-degree in network A and their degree in network B.
Figure 4.9: The time evolution of the values of Additive, Multiplicative, Combined, and Neutral Multiplex PageRank $X$ for the 5 top-ranked users. The damping factors used for the IM and forum network data are $\alpha_A = \alpha_B = 0.85$. Each time step reflects the cumulative interactions in a three-week time window.

Fig. 4.10 does indeed provide support in favor of our hypothesis. Findings thus suggest that the Additive and Multiplicative versions of PageRank can be well approximated by the following two simple measures of centrality for multiplex networks: respectively, the linear combination of nodes' degrees in the different layers, and the multiplication of nodes' degrees in the different layers.

Finally, we found that in our dataset the distribution of Multiplex PageRank is broad, especially the one of the Multiplicative and Combined versions of Multiplex PageRank (See Figure 4.11), as is expected in the case of multiplex networks with positive correlations between degrees of nodes in the different layers.
Figure 4.10: The estimated ranks of users according to the sum \((c_A k_{\text{in}}^A + c_B k^B)\) and product \((k_{\text{in}}^A k^B)\) of their in-degrees and degrees plotted against the values of their Additive and Multiplicative Multiplex PageRank, respectively. In the figure \(c_A = (1 - \alpha_B) \alpha_A / \langle k_{\text{in}}^A \rangle N(x)_B\) and \(c_B = \alpha_B / \langle k^B \rangle\). Note that the node with rank 1 is the most important node of the network, and therefore the Additive and Multiplicative Multiplex PageRanks of the most important nodes of the online social network are correlated, respectively, with a linear combination or the product of the users' in-degrees and degrees.

4.3.5 Concluding Remarks

In conclusion, in this section we introduced Multiplex PageRank, namely a centrality measure that can be used to identify and rank important nodes in multiplex networks. In particular, we defined four versions of this measure: the Additive, Multiplicative, Combined, and Neutral Multiplex PageRank. We then analyzed how these measures correlate with the degree of the nodes in the different layers, both at the mean-field level and using data on an online social network. The empirical application of these measures to our dataset indicated that taking into consideration the multiplex nature of social interaction helps uncover the emergence of rankings of nodes and of structural properties that would otherwise remain undetected if only univariate single networks were investigated.
Figure 4.11: The distribution $P(X)$ of the Additive, Multiplicative, Combined, and Neutral versions of Multiplex PageRank $X$ for users in the IM-forum multiplex network dataset. The damping factors used for the IM and forum data are $\alpha_A = \alpha_B = 0.85$. 

---

Additive ($\beta=0, \gamma=1$)

Multiplicative ($\beta=1, \gamma=0$)

Combined ($\beta=1, \gamma=1$)

Neutral ($\beta=0, \gamma=0$)
Chapter 5

Interacting and Multiplex Spatial Networks – Overlap and Implications on Navigability

Spatial networks, where nodes and links are bound by a geometric space, are a very important class of networks which most real life systems are based on. Moreover, many of these networks are multilayered, interacting with each other or being represented in several different layers. In this final chapter of the thesis, with the aim of reconciling the spatial nature of networks with the emerging theory of multiplex and interacting networks, we build on the statistical mechanics approach for network ensembles and characterize maximal entropy ensembles of interacting and multiplex spatial networks. We first study the local and global overlap of links in multiplex spatial ensembles. We then build ensembles of interacting spatial networks and analyze the dataset of interacting air and railway transportation networks in India in terms of a link probability metric and discuss its implications in navigability.

5.1 Background

The mathematical abstraction of a graph as classically studied in graph theory lacks spatial attributes such as vertices having positions and edges having certain lengths. In real life, however, space is an essential element to many complex systems. Many real-world networks are spatial [239], meaning they are embedded in a real [240–244] or hidden space [245, 246]. The geometric constraints exerted on the system by this spatial em-
beddedness has great impact on both the topology of these networks and the dynamical processes defined on them. For instance, in many spatial networks, there is a wiring cost associated with the length of the link, making it costlier to establish long-range links. Having long-range links is usually justified by some benefit that makes it worth the cost, such as connecting to a high degree node. Important examples of spatial networks are brain networks [240], infrastructures [241,242], road networks [243], and social networks [245]. Moreover, many of these networks are also multiplex indicating that the $N$ nodes of the system can be connected by links of different nature forming a multilayer structure of networks. In transportation networks, two locations can be linked at the same time by a railway connection and a flight connection. In physiology, the brain network interacts with the circulatory system that supplies blood to the brain. In social networks, people can be linked at the same time by friendship, familial or professional ties, etc. Having many areas of application, the framework of multiplex networks has garnered recent attention. New multiplex datasets [193,194,196,247–249] and multiplex network measures have been introduced in order to quantify their complexity. Examples of such measures are the overlap [193,196,249] of links in different layers, the interdependence [248,250] that extends the concept of betweenness centrality to multiplexes, and centrality measures [13,229] for multiplexes (see also Section 4.3). Many dynamical processes have been defined on multiplexes, including cascades of failure in interdependent networks [181,185,251–253], antagonistic percolation [207], dynamical cascades [208], diffusion [188], epidemic spreading [209], election models [12] (see also Section 4.2), game theory [190,254], and so forth. Furthermore, multiplex network models are starting to be proposed following equilibrium or non-equilibrium approaches [199–202]. For instance, it has been shown in [199] that the extension of the configuration model to uncorrelated multiplex networks results in a vanishing overlap in the thermodynamic limit.

In this chapter of the thesis, we contribute to the previous studies on the statistical mechanics of network ensembles [43,44,80,255–258] by characterizing the statistical mechanics of spatial multiplex ensembles. These ensembles of multiplexes can be used for generating multiplexes with given structural properties or for randomizing given spatial multiplex datasets and have potential impact modelling and inference of spatial multiplexes. We demonstrate a noticeable property of spatial multiplexes: these multilayer structures where the nodes are positioned in a real or hidden space naturally allow for the emergence of overlap. This phenomenon can explain why significant overlap is encountered so often in multiplex datasets [193,196,249] and might have important implications
for brain networks, transportation networks, social networks and in general any spatial multiplex. Indeed, the presence of link overlap has been demonstrated to significantly affect the outcome of dynamical processes such as percolation [259, 260].

In Section 5.5, we also study interacting network ensembles where different layers of the complex multilayer structure have disparate set of nodes (with not necessarily the same number of nodes) coupled by interconnections between them. Here, it is worthwhile to note that due to the incredible pace with which the field of multilayered networks is evolving, there is some lack of agreement in the terminology when it comes to naming different types of multilayered networks. What we call interacting networks throughout Section 5.5 to denote networks with disparate sets of nodes interacting via interconnections are sometimes called interconnected networks in literature. We refer the readers interested in the current subtleties in terminology to [7] for an exhaustive list of multilayer network types and their properties. With this definition of interacting networks, we characterize the airport network [261] and the railway network in India, taking the analysis of the railway network in India performed ten years ago [241] one step further. We observe that the airport network and the railway network have different degree distributions and degree correlations. Nevertheless, the function $W(d)$ modulating the link probability with the distance between the nodes decays as a power-law with distance, i.e. $W(d) \propto d^{-\delta}$, for large distances. This indicates that in both networks long distance connections are significantly represented, improving the navigability of the two interacting networks. Moreover, it suggests that these networks can be considered maximal entropy networks associated with a given cost of connection depending logarithmically on the distance between the linked nodes.

5.1.1 Statistical mechanics of networks: The exponential random graph approach

Statistical mechanics has proved to be a very useful tool in the modeling of networks with its rigorous probabilistic arguments and solid theoretical foundations. The goal in modeling a network is usually to achieve an expected characteristic of the network such as degree distribution, degree sequence, clustering coefficient, etc. In the framework of statistical mechanics, the modeling approach is to build network ensembles [43, 44, 80, 255–258], meaning a probability distribution over many network realizations chosen such that the networks with the desired property are represented with a higher probability.
Each network $G = (V, E)$ of the ensemble with the given structural property is assigned a probability $P(G)$. For this ensemble, the entropy $S$ quantifies the logarithm of the typical number of networks represented in the ensemble and is given by

$$
S = - \sum_G P(G) \log P(G). \quad (5.1)
$$

The entropy also quantifies the complexity of the ensemble under consideration. Suppose that we want to construct a network ensemble satisfying a set $K$ of soft constraints (constraints satisfied on average)

$$
\sum_G F_\mu(G) P(G) = C_\mu, \quad (5.2)
$$

with $\mu = 1, 2, \ldots, K$, and $F_\mu(G)$ being a function of the network. For example, $F_\mu(G)$ can be the total number of links or the degree of a node of the network. The least biased way of constructing a network ensemble satisfying these constraints is by maximizing the entropy $S$ given by Eq. (5.1) under the constraints given by Eqs. (5.2). By introducing the Lagrangian multipliers $\lambda_\mu$ and maximizing the entropy, we get that the probability for a network in this network ensemble is given by the exponential

$$
P(G) = \frac{1}{Z} e^{-\sum_{\mu=1}^{K} \lambda_\mu F_\mu(G)}, \quad (5.3)
$$

where $Z$ is the normalization constant, and the values of the Lagrangian multipliers $\lambda_\mu$ for each constraint $\mu = 1, 2, \ldots, K$ are fixed by imposing the constraints in Eqs. (5.2). Due to the exponential form of $P(G)$, this specific type of ensemble is called an exponential random network ensemble. It is also called a canonical network ensemble because the constraints $F_\mu(G)$ are only satisfied on average. If we indicate by $a_{ij}$ the matrix element $(i,j)$ of the adjacency matrix of a generic network in the ensemble, in this ensemble the probability of a link between node $i$ and node $j$ is given by

$$
p_{ij} = \langle a_{ij} \rangle = \sum_G a_{ij} \frac{1}{Z} e^{-\sum_{\mu=1}^{K} \lambda_\mu F_\mu(G)}. \quad (5.4)
$$
5.2 Ensembles of spatial networks

5.2.1 General derivation

In this section, we consider spatial network ensembles where the nodes of each network are embedded in a geometric space with each node \( i = 1, 2, \ldots, N \) positioned at a point of coordinates \( \vec{r}_i \). Subsequently we can define a distance \( d_{ij} \) for each pair of nodes \( i \) and \( j \). The probability of a network in the spatial ensemble is conditioned on the values of the coordinates of the nodes, i.e. strictly speaking we have a \( P(G|\{\vec{r}_i\}) \) where \( \{\vec{r}_i\} \) is the complex set of the coordinates of the nodes in the geometric embedding space. For ensembles of spatial networks the *entropy* \( S \) is given by

\[
S = -\sum_G P(G|\{\vec{r}_i\}) \log P(G|\{\vec{r}_i\}). \tag{5.5}
\]

Spatial network ensembles can be constructed by maximizing the entropy of the ensemble, while fixing a set \( K \) of soft constraints

\[
\sum_G F_\mu(G|\{\vec{r}_i\}) P(G|\{\vec{r}_i\}) = C_\mu, \tag{5.6}
\]

with \( \mu = 1, 2, \ldots, K \), where \( F_\mu(G|\{\vec{r}_i\}) \) is a function of the network and the positions of the nodes. In this way it is easy to show that the probability \( P(G|\{\vec{r}_i\}) \) of a network in this ensembles is given by

\[
P(G|\{\vec{r}_i\}) = \frac{1}{Z} e^{-\sum_{\mu=1}^{K} \lambda_\mu F_\mu(G|\{\vec{r}_i\})}, \tag{5.7}
\]

where \( Z \) is the normalization constant, and the values of the Lagrangian multipliers \( \lambda_\mu \) for each constraint \( \mu = 1, 2, \ldots, K \) are fixed by imposing the constraints in Eqs. (5.6).

5.2.2 Specific examples

5.2.2.1 Spatial network ensemble with fixed expected number of links at a given distance

Maximal entropy network ensembles or exponential random networks are not only interesting in order to model a certain class of networks, but also provide a well defined framework to construct null network models starting from a real network realization [43]. In this context we can also call these ensembles randomized network ensembles. Let us
assume, for example, we have a given undirected spatial network and we want to construct randomized versions of it satisfying a set of constraints. The way to do this is by sampling the maximum entropy ensemble. In the construction of a randomized version of a spatial network, it is interesting to consider in many cases networks satisfying the following constraints at the same time:

- (a) the expected degree sequence in the network ensemble is equal to the degree sequence of the given network;
- (b) the number of expected links connecting nodes at a given distance is equal to the number of such links observed in the given network.

In this case the set of constraints \( F_{\mu}(G|\{r_i\}) \) are given by the following conditions:

- (a) The conditions on the expected degrees can be expressed as
  \[
  \kappa_i = \sum_G P(G|\{r_i\}) F_i(G) = \sum_G P(G|\{r_i\}) \sum_{j=1}^N a_{ij},
  \]
  for \( \mu = i = 1, 2 \ldots, N \) (where \( \kappa_i \) is the expected degree of node \( i \) in the ensemble).

- (b) The conditions on the expected number of links at a given distance can be expressed as
  \[
  n(d_\mu) = \sum_G P(G|\{r_i\}) F_\mu(G|\{r_i\}) = \sum_G P(G|\{r_i\}) \sum_{i<j} a_{ij} \chi_\mu(d_\mu, d_{ij}),
  \]
  where we have discretized the possible range of distances in bins \((d_\mu, d_\mu + \Delta_\mu d)\) with \( \mu = N + 1 \ldots K \). Here, \( \Delta_\mu d \) indicates the size of the \( \mu \)'th bin (for example we can take bins of size increasing as a power-law of the distance \( d_\mu \)). In Eq. (5.9), the function \( \chi_\mu(d_\mu, d_{ij}) \) is such that \( \chi_\mu(d_\mu, d_{ij}) = 1 \) if \( d_{ij} \in (d_\mu, d_\mu + \Delta_\mu d) \) and \( \chi_\mu(d_\mu, d_{ij}) = 0 \) otherwise.
In this spatial network ensemble the probability \( P(G|\{\vec{r}_i\}) \) given by Eq. (5.7) takes on the simple form

\[
P(G|\{\vec{r}_i\}) = \prod_{ij} [p_{ij}(d_{ij})]^{a_{ij}} [1 - p_{ij}(d_{ij})]^{1-a_{ij}}.
\]

(5.10)

with

\[
p_{ij}(d_{ij}) = \frac{e^{-\lambda_i - \lambda_j - \sum_{\mu=N+1,K} \lambda_{\mu} \chi(d_{\mu},d_{ij})}}{1 + e^{-\lambda_i - \lambda_j - \sum_{\mu=N+1,K} \lambda_{\mu} \chi(d_{\mu},d_{ij})}},
\]

(5.11)

where the Lagrangian multipliers \( \lambda_{\mu} \) are fixed by the conditions Eqs. (5.8) – (5.9). Another way to write the link probability in Eq. (5.11) is by setting \( e^{-\lambda_i} = \theta_i \) and \( e^{-\sum_{\mu=N+1,K} \lambda_{\mu} \chi(d_{\mu},d_{ij})} = W(d_{ij}) \) and write

\[
p_{ij}(d_{ij}) = \frac{\theta_i \theta_j W(d_{ij})}{1 + \theta_i \theta_j W(d_{ij})}.
\]

(5.12)

In [80], the network of top 500 USA airports [242] was studied and the function \( W(d) \) was measured from the data. It was shown that this function decays as a power-law of the distance for large distances, i.e. \( W(d) \propto d^{-\delta} \) with \( \delta \approx 3 \) [80] for the dataset under consideration.

5.2.2.2 Spatial network ensemble with fixed expected total cost of the links

As discussed in the Background section, from brain networks to transportation networks, many spatial networks have a cost associated with each link that is usually a function of the distance between the connected nodes. To address this aspect, here we consider network ensembles with the following constraints:

- (a) We fix the expected degree \( \kappa_i \) for each node \( i = 1, 2, \ldots, N \) of the network

\[
\kappa_i = \sum_G P(G|\{\vec{r}_i\}) F_i(G)
\]

\[
= \sum_G P(G|\{\vec{r}_i\}) \sum_{j=1}^N a_{ij},
\]

(5.13)

- (b) Keeping the expected degrees fixed, we also fix the total cost \( L \) of the links. In particular, \( L \) is the sum of all the costs \( f(d_{ij}) \) of the links \( (i, j) \), where we assume
that these costs are a function of the distance \( d_{ij} \) between nodes. Therefore we take

\[
L = \sum_G P(G|\{\vec{r}_i\})F_{N+1}(G|\{\vec{r}_i\})
\]

\[
= \sum_G P(G|\{\vec{r}_i\}) \sum_{i<j} f(d_{ij})a_{ij}.
\] (5.14)

In this spatial network ensemble the probability \( P(G|\{\vec{r}_i\}) \) given by Eq. (5.7) takes the simple form

\[
P(G|\{\vec{r}_i\}) = \prod_{ij} \left[ p_{ij}(d_{ij}) \right]^{a_{ij}} [1 - p_{ij}(d_{ij})]^{1-a_{ij}}.
\] (5.15)

with

\[
p_{ij}(d_{ij}) = \frac{e^{-\lambda_i - \lambda_j - \lambda_{N+1} f(d_{ij})}}{1 + e^{-\lambda_i - \lambda_j - \lambda_{N+1} f(d_{ij})}}.
\] (5.16)

The function \( f(d) \) can be chosen arbitrarily. Typical functions that can be considered include the distance, and the logarithm of the distance, i.e.

\[
f(d_{ij}) = d_{ij}
\] (5.17)

\[
f(d_{ij}) = \log d_{ij}.
\] (5.18)

These two expressions lead respectively to the following probabilities of having a link between node \( i \) and node \( j \).

\[
p_{ij}(d_{ij}) = \frac{e^{-\lambda_i - \lambda_j - d_{ij}/d_0}}{1 + e^{-\lambda_i - \lambda_j - d_{ij}/d_0}}
\] (5.19)

\[
p_{ij}(d_{ij}) = \frac{e^{-\lambda_i - \lambda_j} d_{ij}^{-\delta}}{1 + e^{-\lambda_i - \lambda_j} d_{ij}^{-\delta}}
\] (5.20)

where the \( N + 1^{th} \) Lagrangian multiplier enforcing the constraint Eq.(5.14) is given by \( \lambda_{N+1} = 1/d_0 \) in the first case and \( \lambda_{N+1} = \delta \) in the second case. The Lagrangian multipliers \( \lambda_i \) with \( i = 1, 2 \ldots, N \) enforce the conditions over the expected degree of the node \( i \). The
probabilities Eq. (5.19) and Eq. (5.20) can also be expressed in terms of \( \theta_i = e^{-\lambda_i} \), i.e.

\[
\begin{align*}
\rho_{ij}(d_{ij}) &= \frac{\theta_i \theta_j e^{-d_{ij}/d_0}}{1 + \theta_i \theta_j e^{-d_{ij}/d_0}} \\
\rho_{ij}(d_{ij}) &= \frac{\theta_i \theta_j d_{ij}^{-\delta}}{1 + \theta_i \theta_j d_{ij}^{-\delta}}
\end{align*}
\]

(5.21)

(5.22)

where \((\{\theta_i\}, d_0)\) or \((\{\theta_i\}, \delta)\) are called “hidden variables”. Therefore if we analyze a real network dataset considering the randomized network ensemble with expected number of links at a given distance (as we have done in the previous subsection) and we observe a probability distribution given by Eq. (5.12) with \( W(d) \propto d^{-\delta} \), we can deduce that the network can be thought of as maximal entropy network with an associated cost of the links given by Eqs. (5.14), (5.18). On the other hand, if we observe \( W(d) \propto e^{-d/d_0} \) the network ensemble can be thought of as a maximal entropy network ensemble with an associated cost of the links given by Eqs. (5.14), (5.17).

### 5.2.2.3 Spatial bipartite network ensemble with fixed expected number of links at a given distance

Spatial networks can be of different types: directed, weighted, with nodes having features, etc. An interesting case that we will consider here is the one in which the spatial network is bipartite. To this end, we will define maximal entropy ensembles of bipartite spatial networks. Let us suppose that \( b_{ij} \) is the incidence matrix of the bipartite network, with \( i = 1, 2, \ldots, N_1 \) and \( j = 1, 2, \ldots, N_2 \) indicating distinct nodes of coordinates \( \{\vec{r}_1^i\} \) and \( \{\vec{r}_2^j\} \), respectively.

As an example of a bipartite spatial network ensemble, we consider the network in which we fix the expected degree \( \{\kappa_1^i\} \) of nodes \( i = 1, 2, \ldots, N_1 \) and the expected degree \( \{\kappa_2^j\} \) of nodes \( j = 1, 2, \ldots, N_2 \), in addition to which we fix the expected number of links at a given distance \( n(d_\mu) \). The soft constraints that we impose on the ensemble are thus given by the following list:

- (a) The conditions on the expected average degrees \( \{\kappa_1^i\} \) can be expressed as

\[
\kappa_1^i = \sum_G P(G|\{\vec{r}_1^i\}, \{\vec{r}_2^j\}) \sum_{j=1}^{N_2} b_{ij},
\]

(5.23)

for \( i = 1, 2, \ldots, N_1 \). These are the conditions \( \mu = 1, 2, \ldots, N_1 \).
• (b) The conditions on the expected average degrees \( \{ \kappa_j^2 \} \) can be expressed as

\[
\kappa_j^2 = \sum_G P(G|\{r_i^1\},\{r_j^2\}) \sum_{i=1}^{N_1} b_{ij},
\]

(5.24)

for \( j = 1, 2, \ldots, N_2 \). These are the conditions \( \mu = N_1 + 1, \ldots, N_1 + N_2 \).

• (c) The conditions on the expected number of nodes at a given distance can be expressed as

\[
n(d_\mu) = \sum_G P(G|\{r_i^1\},\{r_j^2\}) \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} b_{ij} \chi_\mu(d_\mu, d_{ij}),
\]

(5.25)

where we have discretized the possible range of distances in bins \( (d_\mu, d_\mu + \Delta_\mu d) \) with \( \mu = N_1 + 1, \ldots, K \). Once again, we have that \( \chi_\mu(d_\mu, d_{ij}) = 1 \) if \( d_{ij} \in (d_\mu, d_\mu + \Delta_\mu d) \) and \( \chi_\mu(d_\mu, d_{ij}) = 0 \) otherwise.

Following the same approach described in the previous cases, we can show that

\[
P(G|\{r_i^1\},\{r_j^2\}) = \prod_{ij} [p_{ij}(d_{ij})]^{b_{ij}} [1 - p_{ij}(d_{ij})]^{1-b_{ij}}.
\]

(5.26)

with

\[
p_{ij}(d_{ij}) = \frac{e^{-\lambda_i - \lambda_{N_1} - j - \sum_{\mu=N_1+N_2+1,K} \lambda_\mu \chi(d_\mu, d_{ij})}}{1 + e^{-\lambda_i - \lambda_{N_1} - j - \sum_{\mu=N_1+N_2+1,K} \lambda_\mu \chi(d_\mu, d_{ij})}},
\]

(5.27)

where the Lagrangian multipliers \( \lambda_\mu \) are fixed by the conditions given in Eqs. (5.23), (5.24), (5.25).

Another way to write the link probability in Eq. (5.27) is by setting \( e^{-\lambda_i} = \theta_i^1 \) and \( e^{-\sum_{\mu=N_1+N_2+1,K} \lambda_\mu \chi(d_\mu, d_{ij})} = W(d_{ij}) \), which results in the expression

\[
p_{ij}(d_{ij}) = \frac{\theta_i^1 \theta_j^2 W(d_{ij})}{1 + \theta_i^1 \theta_j^2 W(d_{ij})}.
\]

(5.28)

### 5.3 Ensembles of multiplex networks

A multiplex is a multilayer structure formed by \( M \) layers and \( N \) nodes \( i = 1, 2, \ldots, N \). Every node is represented in every layer of the multiplex. Every layer \( \alpha = 1, 2, \ldots, M \) is formed by a network \( G_\alpha = (V_\alpha, E_\alpha) \) with adjacency matrix of elements \( a_{ij}^{\alpha} = 1 \) if there is a link between node \( i \) and node \( j \) in layer \( \alpha \) and \( a_{ij}^{\alpha} = 0 \) otherwise.
5.3.1 Overlap of links in multiplexes

One of the major structural characteristics of a multiplex observed in several datasets is the overlap of links [193, 196, 249]. In this section, we present the definition of global and local overlap of links.

For two layers $\alpha, \alpha'$ of the multiplex, the global overlap $O^{\alpha,\alpha'}$ is defined as the total number of pairs of nodes connected at the same time by a link in layer $\alpha$ and a link in layer $\alpha'$, i.e.

$$O^{\alpha,\alpha'} = \sum_{i<j} a_{ij}^\alpha a_{ij}^{\alpha'}.$$  \hfill (5.29)

On the other hand, for a node $i$ of the multiplex, the local overlap $o_i^{\alpha,\alpha'}$ of links in the two layers $\alpha$ and $\alpha'$ is defined as the total number of nodes $j$ linked to the node $i$ both by a link in layer $\alpha$ and a link in layer $\alpha'$, i.e.

$$o_i^{\alpha,\alpha'} = \sum_{j=1}^N a_{ij}^\alpha a_{ij}^{\alpha'}.$$  \hfill (5.30)

We expect the global and local overlap in spatial networks to be significant. For example, in transportation networks within the same country, if we consider train and long-distance bus transportation, we expect to observe a significant overlap. Also in case of social multiplex networks where each layer represents a different means of communication between people (emails, mobile, text messaging, etc.), two people that are linked in one layer are also likely to be linked in another layer, forming a multiplex with significant overlap. This observation is supported by the analysis of real multiplex datasets [193, 196, 249] that display a significant overlap of links.

5.3.2 Multiplex ensembles

Multiplex ensembles describe ensembles of maximal entropy multiplexes satisfying specific structural constraints, and are proposed to be very efficient null models for describing real multiplexes with different features. A multiplex ensemble is determined once the probability $P(\vec{G})$ of the multiplex $\vec{G} = (G^1, G^2, \ldots, G^\alpha, \ldots, G^M)$ is fixed. The entropy of the multiplex ensemble $S$ is given by

$$S = - \sum_{\{\vec{G}\}} P(\vec{G}) \log P(\vec{G}).$$  \hfill (5.31)
and maximum entropy multiplex ensembles can be defined as a function of the soft constraints we plan to impose on the ensemble [199]. We assume having $K$ of such constraints determined by the conditions

$$\sum_{\tilde{G}} P(\tilde{G}) F_\mu(\tilde{G}) = C_\mu$$

(5.32)

with $\mu = 1, 2 \ldots, K$ where $F_\mu(\tilde{G})$ determines the structural constraints that we want to impose on the multiplex. For example, $F_\mu(\tilde{G})$ can be equal to the total number of links in a layer of the multiplex $\tilde{G}$ or the degree of a node in a layer of the multiplex $\tilde{G}$ (for a detailed account see [199]). Maximizing the entropy given by Eq. (5.31) while satisfying the constraints given by Eqs. (5.32), we find that the probability of a multiplex $P(\tilde{G})$ in the multiplex ensemble is given by

$$P(\tilde{G}) = \frac{1}{Z} \exp \left[ - \sum_\mu \lambda_\mu F_\mu(\tilde{G}) \right],$$

(5.33)

where $Z$ is the normalization constant, and the Lagrangian multipliers $\lambda_\mu$ are fixed by the constraints in Eqs. (5.32).

### 5.3.3 Uncorrelated multiplex ensembles and their overlap

Uncorrelated multiplex ensembles have a probability $P(\tilde{G})$ that can be factorized into the probability of single networks, i.e.

$$P(\tilde{G}) = \prod_{\alpha=1}^M P_\alpha(G_\alpha).$$

(5.34)

These ensembles are maximal entropy multiplex ensembles in which every soft constraint involves just a single network. Furthermore in many cases the constraints are linear in the adjacency matrix. Examples of such constraints are the cases in which we fix the expected degree sequence, or the number of nodes between communities. In these cases the probability $P_\alpha(G_\alpha)$ takes on the simple expression

$$P_\alpha(G_\alpha) = \prod_{i<j} \left[ p_{ij}^\alpha a_{ij} + (1 - p_{ij}^\alpha)(1 - a_{ij}) \right].$$

(5.35)

An important example of such multiplexes is the one in which we fix the expected degree $\kappa_i^\alpha$ of each node $i$ in each layer $\alpha$ and we impose the structural cutoff $\kappa_i^\alpha < \sqrt{\langle \kappa^\alpha \rangle N}$. In
In this case we have

\[ p_{ij}^{\alpha} = \frac{\kappa_i^{\alpha} \kappa_j^{\alpha}}{\langle \kappa^{\alpha} \rangle N}. \]  

(5.36)

If the multiplex ensemble is uncorrelated and \( P_{\alpha}(G_{\alpha}) \) is given by Eq. (5.35), we can easily calculate the average global overlap \( \langle O^{\alpha,\alpha'} \rangle \) and the average local overlap \( \langle o_i^{\alpha,\alpha'} \rangle \) between two layers \( \alpha \) and \( \alpha' \), where the global overlap \( O^{\alpha,\alpha'} \) is defined in Eq. (5.29) and the local overlap \( o_i^{\alpha,\alpha'} \) is defined in Eq. (5.30). These quantities are given by

\[
\langle O^{\alpha,\alpha'} \rangle = \sum_{i<j} p_{ij}^{\alpha} p_{ij}^{\alpha'}
\]

\[
\langle o_i^{\alpha,\alpha'} \rangle = \sum_{j=1, j \neq i}^{N} p_{ij}^{\alpha} p_{ij}^{\alpha'}.
\]  

(5.37)

For multiplex ensembles with given expected degree of the nodes in each layer, with \( p_{ij}^{\alpha} \) given by Eq. (5.36) we have

\[
\langle O^{\alpha,\alpha'} \rangle = \frac{1}{2} \left( \frac{\langle \kappa_i^{\alpha} \kappa_j^{\alpha'} \rangle^2}{\langle \kappa^{\alpha} \rangle \langle \kappa^{\alpha'} \rangle} \right)
\]

\[
\langle o_i^{\alpha,\alpha'} \rangle = \kappa_i^{\alpha} \kappa'_i \frac{\langle \kappa_i^{\alpha} \kappa_i^{\alpha'} \rangle}{\langle \kappa^{\alpha} \rangle \langle \kappa^{\alpha'} \rangle N}
\]  

(5.38)

where \( \langle \kappa^{\alpha} \kappa^{\alpha'} \rangle = \sum_{i=1}^{N} \kappa_i^{\alpha} \kappa_i^{\alpha'}/N \).

If the expected degrees in the different layers are uncorrelated (i.e. \( \langle \kappa^{\alpha} \kappa^{\alpha'} \rangle = \langle \kappa^{\alpha} \rangle \langle \kappa^{\alpha'} \rangle \)) then the global and local overlaps are given by

\[
\langle O^{\alpha,\alpha'} \rangle = \frac{1}{2} \left( \langle \kappa^{\alpha} \rangle \langle \kappa^{\alpha'} \rangle \right) \ll N
\]

\[
\langle o_i^{\alpha,\alpha'} \rangle = \kappa_i^{\alpha} \kappa'_i \frac{\langle \kappa_i^{\alpha} \kappa_i^{\alpha'} \rangle}{N} \ll \min(\kappa_i^{\alpha}, \kappa_i^{\alpha'})
\]  

(5.39)

Therefore in this case the overlap is negligible. Degree correlations between different layers can enhance the overlap, but as long as \( \langle \kappa^{\alpha} \kappa^{\alpha'} \rangle \ll N \), the average global overlap \( \langle O^{\alpha,\alpha'} \rangle \) and the local overlap \( \langle o_i^{\alpha,\alpha'} \rangle \) will continue to be negligible compared to the total number of nodes in the two layers and the degrees of the node \( i \) in the two layers, respectively. Similarly, the expected global and local overlap are both negligible in the multiplex ensemble.
in which we fix the average degree of each node in each layer and the average number of links between nodes of different communities in each layer. In general, as long as we have an uncorrelated multiplex with \( P_\alpha(G_\alpha) \) given by Eq. (5.35) and \( p^\alpha_{ij} \ll 1, \forall (i,j) \), then the expected local and global overlap is negligible. The way to solve this problem is to consider correlated multiplexes. It is possible to model multiplexes with a given set of multilinks, as described in [199]. However, it is also possible to consider spatial multiplexes, as we discuss in the following section.

5.4 Ensembles of multiplex spatial networks

5.4.1 General derivation

In multiplex spatial networks \( \vec{G} = (G_1, G_2, \ldots, G_M) \) where \( M \) is the number of layers in the multiplex, each layer \( G_\alpha = (V, E_\alpha) \) with \( \alpha = 1, 2, \ldots, M \) is formed by the same \( N \) nodes embedded in a metric space. Each node \( i \) is assigned a coordinate \( \vec{r}_i \) in this metric space. A spatial multiplex ensemble is defined once we define the probability \( P(\vec{G}|\{\vec{r}_i\}) \) of the multiplex \( \vec{G} \) conditioned on the positions of the nodes \( \{\vec{r}_i\} \). For ensembles of spatial multiplexes the entropy \( S \) is given by

\[
S = -\sum_{\vec{G}} P(\vec{G}|\{\vec{r}_i\}) \log P(\vec{G}|\{\vec{r}_i\}).
\]  

(5.40)

As we did in the previous sections, we can construct spatial multiplex ensembles by maximizing the entropy of the ensemble, while fixing a set \( K \) of soft constraints

\[
\sum_{\vec{G}} P(\vec{G}|\{\vec{r}_i\}) F_\mu(\vec{G}|\{\vec{r}_i\}) = C_\mu,
\]  

(5.41)

with \( \mu = 1, 2, \ldots, K \), and \( F_\mu(\vec{G}|\{\vec{r}_i\}) \) being a function of the multiplex and the positions of the nodes. Hence, we get that the probability \( P(\vec{G}|\{\vec{r}_i\}) \) of a multiplex in this ensemble is given by

\[
P(\vec{G}|\{\vec{r}_i\}) = \frac{1}{Z} e^{-\sum_{\mu=1}^{K} \lambda_\mu F_\mu(\vec{G}|\{\vec{r}_i\})},
\]  

(5.42)

where \( Z \) is the normalization constant, and the values of the Lagrangian multipliers \( \lambda_\mu \) for each constraint \( \mu = 1, 2, \ldots, K \) are fixed by imposing the constraints in Eqs. (5.41). A particular case of a spatial multiplex ensemble is generated by this approach when each
constraint $F_\mu(\bar{G}|\{\vec{r}_i\})$ involves a single network in one layer of the multiplex. In this case $P(\bar{G}|\{\vec{r}_i\})$ can be written as

$$P(\bar{G}|\{\vec{r}_i\}) = \prod_{\alpha=1}^{M} P_\alpha(G_\alpha|\{\vec{r}_i\}).$$  \hspace{1cm} (5.43)

One should note that in this case the multiplex is not uncorrelated because the probabilities $P_\alpha(G_\alpha|\{\vec{r}_i\})$ appearing in Eq. (5.43) are conditioned on the position of the nodes $\{\vec{r}_i\}$ that are the same for every network $\alpha$. In particular, unlike the case in which we have Eq. (5.34), these types of spatial multiplexes might show a significant overlap of the links. We shall demonstrate this feature in the following section.

### 5.4.2 Expected overlap of spatial multiplexes

As we mentioned previously in the chapter, many spatial multiplexes naturally develop a significant overlap. For simplicity, let us consider spatial multiplex ensembles in which every multiplex has a probability given by Eq. (5.43) where the probabilities $P_\alpha(G_\alpha|\{\vec{r}_i\})$ are given by Eq. (5.7). The goal of this section is to show that these multiplexes, unlike uncorrelated multiplexes satisfying Eq. (5.34) can have a significant overlap. In the following, we will focus on multiplex ensembles with link probability decaying exponentially with distance and we will refer the interested reader to the appendix for the generalization of this derivation to multiplexes with links decaying as a power-law of the distance or with different layers characterized by different spatial behavior, i.e. some layers with link probability decaying exponentially with distance and some layers with link probability decaying as a power-law of the distance.

#### 5.4.2.1 Multiplex ensembles with link probability decaying exponentially with distance

Here we evaluate the expected overlap for a multiplex where each $P_\alpha(G_\alpha|\{\vec{r}_i\})$ is given by Eq. (5.15) that we rewrite here for convenience,

$$P_\alpha(G_\alpha|\{\vec{r}_i\}) = \prod_{i<j} \left[ p_{ij}^\alpha(d_{ij})a_{ij}^{\alpha} + (1 - p_{ij}^\alpha(d_{ij}))(1 - a_{ij}^{\alpha}) \right]$$  \hspace{1cm} (5.44)
where \( p_{ij}^{\alpha}(d_{ij}) \) is given by Eq. (5.21), i.e.

\[
p_{ij}^{\alpha}(d_{ij}) = \frac{\theta_i^\alpha \theta_j^\alpha e^{-d_{ij}/d_{\alpha}}}{1 + \theta_i^\alpha \theta_j^\alpha e^{-d_{ij}/d_{\alpha}}}.
\]  

The “hidden variables” \( \theta_i^\alpha \) fix the expected degree of node \( i \) in layer \( \alpha \), i.e.

\[
k_i^{\alpha} = \sum_j p_{ij}^{\alpha}(d_{ij}),
\]

while the “hidden variables” \( d_{\alpha} \) fix the total cost \( L^{\alpha} = N \ell^\alpha \) associated with the links in layer \( \alpha \) given by

\[
L^{\alpha} = N \ell^\alpha = \sum_{i<j} d_{ij} p_{ij}^{\alpha}(d_{ij}).
\]

In these multiplexes the expected total overlap \( \langle O^{\alpha,\alpha'} \rangle \) of the links between layer \( \alpha \) and layer \( \alpha' \) and the expected local overlap \( \langle o_i^{\alpha,\alpha'} \rangle \) of the links between layer \( \alpha \) and layer \( \alpha' \) are given by Eqs. (5.37), which we rewrite here for convenience,

\[
\langle O^{\alpha,\alpha'} \rangle = \sum_{i<j} p_{ij}^{\alpha} p_{ij}^{\alpha'}
\]

\[
\langle o_i^{\alpha,\alpha'} \rangle = \sum_{j=1,j\neq i}^N p_{ij}^{\alpha} p_{ij}^{\alpha'}.
\]

Here we want to show that the expected total and local overlap can be significant for the spatial multiplex ensemble under consideration.

Let us for simplicity consider a multiplex in which the expected degrees in a certain layer are all equal and finite. Moreover, let us assume that the nodes are distributed uniformly on a \( D \) dimensional Euclidean hypersphere of radius \( R \), with density \( \rho \). Therefore, we have \( k_i^{\alpha} = k^\alpha \ \forall i \) and the hidden variables in a given layer are the same for every node, i.e. \( \theta_i^\alpha = \theta^\alpha \ \forall i \). Thus we can estimate the relation between \( (k^\alpha, L^\alpha) \) and \( (\theta^\alpha, d_{\alpha}) \). Approximating the sum over \( j \) with an integral over a continuous distribution of points in
Eq. (5.46), we find

\begin{align*}
\kappa^{\alpha} & \simeq \rho \Omega(D) \int_{0}^{R} dr \ r^{D-1} \frac{(\theta^{\alpha})^2 e^{-r/d_{\alpha}}}{1 + (\theta^{\alpha})^2 e^{-r/d_{\alpha}}} \\
& \simeq \rho \Omega(D) \sum_{n=0}^{\infty} (-1)^n \frac{(\theta^{\alpha})^{2(n+1)}}{1 + (\theta^{\alpha})^{2(n+1)}} \int_{0}^{R} dr \ r^{D-1} e^{-r(1+n)/d_{\alpha}} \\
& \simeq \rho \Omega(D) \Gamma(D) d_{\alpha}^{D} \sum_{n=0}^{\infty} (-1)^n \frac{(\theta^{\alpha})^{2(n+1)}}{(1+n)^{D}}, \quad (5.49)
\end{align*}

where \( \Omega(D) \) is the surface area of a \( D \) dimensional hypersphere of radius \( r \) and therefore the solid angle \( \Omega(D) \) is given by \( \Omega(D) = \frac{2\pi^{D/2}}{\Gamma(D/2)} \), and where we have assumed \( \theta^{\alpha} e^{-r/d} < 1 \). Moreover in the large network limit we assume that \( \Omega(D) R^{D}/D \simeq N \) and in the last expression of Eqs. (5.49) we have performed the limit \( R \to \infty \). The relation between \( \kappa^{\alpha} \) and \( (\theta^{\alpha},d_{\alpha}) \) can be further simplified as

\begin{equation}
\kappa^{\alpha} \simeq -\rho \Omega(D) \Gamma(D) d_{\alpha}^{D} \text{Li}_D \left[-(\theta^{\alpha})^2\right], \quad (5.50)
\end{equation}

where \( \text{Li}_n(z) \) is the polylogarithmic function. Performing similar calculations we can show that in the continuous approximation, where we approximate the sum on \( (i,j) \) with an integral over space, we have that Eq. (5.47) can be written as

\begin{equation}
\frac{\ell^{\alpha}}{N} = \frac{1}{2} \ell^{\alpha} \simeq \rho \Omega(D + 1) \Gamma(D + 1) d_{\alpha}^{D+1} \text{Li}_{D+1} \left[-(\theta^{\alpha})^2\right]. \quad (5.51)
\end{equation}

Since we are interested in the case where both \( \kappa^{\alpha} \) and \( \ell^{\alpha} \) are finite, it follows from the Eqs. (5.50) – (5.51), that the “hidden variables” \( (\theta^{\alpha},d_{\alpha}) \) are also finite, i.e. they do not depend on \( N \) in the limit \( N \to \infty \). We can now easily evaluate the scaling with the total number of nodes \( N \) of the expected total overlap between two layers \( \langle O^{\alpha,\alpha'} \rangle \) and the expected local overlap \( \langle o^{\alpha,\alpha'} \rangle \) between two layers using Eqs. (5.48). In particular we have in the continuous approximation, for the expected global overlap between layer \( \alpha \) and layers \( \alpha' \),

\begin{equation}
\langle O^{\alpha,\alpha'} \rangle \simeq N \rho \frac{\Omega(D)}{2} \int_{0}^{R} drr^{D-1} \frac{(\theta^{\alpha})^2 e^{-r/d_{\alpha}}}{1 + (\theta^{\alpha})^2 e^{-r/d_{\alpha}}} \times \frac{(\theta^{\alpha'})^2 e^{-r/d_{\alpha'}}}{1 + (\theta^{\alpha'})^2 e^{-r/d_{\alpha'}}}. \quad (5.52)
\end{equation}

Performing straightforward calculations we get that

\begin{equation}
\langle O^{\alpha,\alpha'} \rangle \simeq N \rho \frac{\Omega(D)}{2} I(\alpha,\alpha') \quad (5.53)
\end{equation}

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where $I(\alpha, \alpha')$ is finite and in the limit $R, N \to \infty$ and is given by

$$I(\alpha, \alpha') \simeq \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (-1)^{m+n} (\theta^\alpha)^{2(n+1)} (\theta^\alpha')^{2(m+1)} \times \left( \frac{d_\alpha d_{\alpha'}}{d_{\alpha'}(1+n) + d_\alpha(1+m)} \right)^D.$$  

(5.54)

Therefore the expected global overlap between two layers is linear in $N$, meaning that a finite fraction of all the links is overlapping. Furthermore, it can be shown that the overlap is significant (finite) in every region of the network, as the expected local overlap is also significant. Indeed, following similar steps used to estimate the expected global overlap, we can show that

$$\langle o_{i}^{\alpha,\alpha'} \rangle \simeq \rho \Omega(D) I(\alpha, \alpha')$$  

(5.55)

with $I(\alpha, \alpha')$ given by Eq. (5.54) in the limit $R, N \to \infty$. These results remain qualitatively the same if the multiplex is formed by networks with heterogeneous degree distributions.

5.5 Interacting spatial networks

5.5.1 Ensembles of interacting networks

The subject of this section is interacting networks which are formed by layers of networks of different nature, and a set of interconnecting nodes between them. An example of interacting networks, we will study the interacting air and railway transportation networks in India, where airports and train stations are usually distinct. In interacting networks, we consider a set of $M$ networks $G_\alpha = (V_\alpha, E_\alpha)$ with $\alpha = 1, 2, \ldots, M$ where the set of nodes $V_\alpha$ is different for every network. In addition to this, we have to take into account the interactions between the nodes in different networks. These interactions can be represented by a set of bipartite networks such as $G_{\alpha, \beta} = (V_\alpha \cup V_\beta, E_{\alpha, \beta})$ that connects the nodes of a network $\alpha$ with the nodes of another network $\beta$. Therefore an ensemble of interacting networks will be given by the set $(\tilde{G}, \tilde{G}) = \{G_\alpha\}, \{G_{\alpha, \beta}\})$. In these types of networks we can have that one node $i$ in network $\alpha$ is linked to several nodes in network $\beta$, or that one node in network $\alpha$ is not linked to any node in network $\beta$. This feature provides a further flexibility of interacting networks with respect to multiplexes where each node of the network is represented at the same time in different layers. As a future direction, it would be very interesting, for instance, to study diffusion processes on interacting networks,
extending the work done for multiplex networks in [188], as well as to investigate other dynamical processes on them.

5.5.2 Ensembles of interacting spatial networks

The statistical mechanical treatment of interacting spatial networks is very similar to that of multiplex spatial networks. Interacting spatial network ensembles are ensembles of networks \((\vec{G}, \vec{G}) = \{G_\alpha, G_{\alpha,\beta}\}\). Each network \(G_\alpha = (V_\alpha, E_\alpha)\) with \(\alpha = 1, 2, \ldots, M\) is formed by a different set of \(N_\alpha\) nodes embedded in a metric space. Each node is assigned a coordinate \(\vec{r}\) in this metric space. Each bipartite network \(G_{\alpha,\beta}\) connects nodes of network \(\alpha\) with nodes of network \(\beta\). In general, an ensemble of interacting spatial networks is defined once we define the probability \(P(\vec{G}, \vec{G}|\{\vec{r}\})\) of having interacting networks \((\vec{G}, \vec{G})\) conditioned on the positions of the nodes \(\{\vec{r}\}\). For ensembles of interacting spatial networks, the entropy \(S\) is given by

\[
S = -\sum_{\vec{G}, \vec{G}} P(\vec{G}, \vec{G}|\{\vec{r}\}) \log P(\vec{G}, \vec{G}|\{\vec{r}\}).
\]  

(5.56)

Interacting spatial network ensembles can be constructed by maximizing the entropy of the ensemble, while fixing a set \(K\) of soft constraints

\[
\sum_{\vec{G}, \vec{G}} P(\vec{G}, \vec{G}|\{\vec{r}\}) F_\mu(\vec{G}, \vec{G}|\{\vec{r}\}) = C_\mu,
\]  

(5.57)

with \(\mu = 1, 2, \ldots, K\), and \(F_\mu(\vec{G}, \vec{G}|\{\vec{r}\})\) being a function of the multiplex and the positions of the nodes. Once again, maximizing the entropy we get that the probability \(P(\vec{G}, \vec{G}|\{\vec{r}\})\) of a multiplex in this ensemble is given by

\[
P(\vec{G}, \vec{G}|\{\vec{r}\}) = \frac{1}{Z} e^{-\sum_{\mu=1}^{K} \lambda_\mu F_\mu(\vec{G}, \vec{G}|\{\vec{r}\})},
\]  

(5.58)

where \(Z\) is the normalization constant, and the values of the Lagrangian multipliers \(\lambda_\mu\) for each constraint \(\mu = 1, 2, \ldots, K\) are fixed by imposing the constraints in Eqs. (5.57). Here we consider the special case of interacting spatial network ensembles generated by the maximal entropy approach when each constraint \(F_\mu(\vec{G}, \vec{G}|\{\vec{r}\})\) involves a single network. In this case \(P(\vec{G}, \vec{G}|\{\vec{r}\})\) can be decomposed as

\[
P(\vec{G}, \vec{G}|\{\vec{r}\}) = \prod_{\alpha=1}^{M} P_\alpha G_\alpha|\{\vec{r}\}\prod_{\alpha<\beta} P_{\alpha,\beta} G_{\alpha,\beta}|\{\vec{r}\}.
\]  

(5.59)
where \( P_\alpha(G_\alpha|\{\vec{r}\}) \) is the probability of a network \( G_\alpha \) in the maximal entropy ensemble and \( P_{\alpha,\beta}(G_{\alpha,\beta}|\{\vec{r}\}) \) is the probability of a bipartite network \( G_{\alpha,\beta} \) in the maximal entropy ensemble.

5.5.3 A case study: The interacting air and railway transportation networks of India

In this part, we investigate the air and railway transportation networks in India as an example of interacting networks. We have extracted the data of train stations and routes and schedules of trains at different stations in the Indian railway network\(^1\). Two stations are connected if there exists a physical track connecting the two stations, with the links corresponding to connections within one stop distance. There are 7408 stations and 13230 links in the railway network. The airport network is generated by establishing links between airports with direct flight connections between them. The data for flight schedules has been extracted from the database of Indian airports\(^2\). In our dataset we have 78 airports with 203 links. Additionally we access the data of the bipartite network of interconnections between airports and train stations from the website indiarailinfo.com. For the purposes of this study, we have accessed only those airports which are commercially used for passenger travel and we have extracted the information about railway stations and nearby airports. The information about a nearby airport is provided if road access is available between the train station and the airport. There are 6769 stations and 102 airports mentioned in the database of interconnections between airports and train stations, out of which 78 airports are commercially used. We therefore drop the remaining 24 airports from our analysis. Additionally we have accessed the latitude and longitude of the airports and of the railway stations using Google maps. In Figure 5.1, we plot the geographic coordinates of the trains station and airport networks under consideration.

In summary, our dataset of interacting networks is formed by the airport network (the AA network) and the railway network (the RR network) of India, and the bipartite network of interconnections between airports and train stations (the AR network). The cumulative degree distributions of the railway network (RR), the airport network (AA) and the airport degree distribution in the AR network are shown in Figure 5.2. We note that the degree distribution of the AA network is broad while the degree distribution of RR is not. Interestingly enough, the degree distribution of the airports in the AR network

\(^1\)www.indianrail.gov.in
\(^2\)www.ourairports.com
Figure 5.1: Map of the Indian railway network (RR) (panel A) and map of the Indian airport network (AA) (panel B).
Figure 5.2: Cumulative degree distribution of the railway network (RR) and the airport network (AA) of India, and the cumulative degree distribution of the airports in the AR bipartite network between airports and railway stations.

is also broad. It is also worth mentioning that the degrees of the railway stations in the AR interconnection network are either one or zero leading to a trivial degree distribution.

The degree correlations in the two interacting networks AA and RR are very different. In order to show this, we plot in Figure 5.3 the function \( k_{nn}(k) \), also called the average degree of the neighbors of a node of degree \( k \), defined as

\[
k_{nn}(k) = \frac{1}{NP(k)} \sum_{i|k_i=k} \sum_j a_{ij}^\alpha k_j, \tag{5.60}
\]

for network AA (\( \alpha = 1 \)) and for network RR (\( \alpha = 2 \)). While the railway network RR is assortative, meaning that it is characterized by an increasing function \( k_{nn}(k) \), the airport network AA is disassortative, meaning it is characterized by a decreasing function \( k_{nn}(k) \). In other words, highly connected airports tend to be linked to low connectivity airports while highly connected railway stations are more likely to be connected to highly connected railway stations. Moreover, in order to characterize other types of correlations, we measure
the Pearson’s correlation coefficient $\rho$ between the degree $k^{AA}$ of an airport in the AA network and the degree $k^{AR}$ of the same airport in the AR network, i.e.

$$\rho = \frac{\langle k^{AA}k^{AR} \rangle - \langle k^{AA} \rangle \langle k^{AR} \rangle}{\sqrt{\langle (k^{AA})^2 \rangle - \langle k^{AA} \rangle^2} \sqrt{\langle (k^{AR})^2 \rangle - \langle k^{AR} \rangle^2}}.$$  \hspace{1cm} (5.61)

The calculated Pearson coefficient is $\rho = 0.3998$ indicating that the degree of airports in the AA network is correlated with the degree of airports in the AR network, enhancing the importance and centrality of high degree airports in this set of interacting networks of air and railway transportation in India.

Finally we consider the ensemble of interacting networks with $M = 2$ where the probability is such that

$$P(G_1, G_2, G_{12}) = P_1(G_1 | \{r\}) P_2(G_2 | \{r\}) P_{12}(G_{12} | \{r\}).$$  \hspace{1cm} (5.62)

The probabilities $P_{1,2}(G_{1,2} | \{r\})$ are the probabilities of spatial networks in which (a) the expected degree of each node is equal to the one observed in the AA network and
the RR network, respectively and (b) the expected average number of links at a given distance is equal to the one observed in the AA network and the RR network, respectively. The probability $P_{12}(G_{12} | \{\vec{r}\})$ is the probability of a bipartite network in the ensemble of bipartite networks where (a) the expected degree of every node is equal to the one observed in the AR network and (b) the expected number of links at a given distance is equal to the one observed in the AR network. In particular, the link probabilities within each layer are given by Eq. (5.12) and the link probabilities in the bipartite network are given by Eq (5.28). In Figure 5.4 we plot the function $W(d)$ (derived in Eq. (5.12), (5.28)), which depends on the distance between the nodes and affects the link probabilities, for the networks AA, RR and AR. We show that the function $W(d)$ at large distances decays as a power-law $W(d) \propto d^{-\delta}$ for the three cases under consideration and we indicate the fitted values of the exponents $\delta$ in the Figure 5.4. This shows that all these networks allow for long-range connections and therefore the entire interacting network displays a good navigability. We notice that the railway network (the RR network) is characterized by a $\delta$ exponent roughly half of that of the airport network (the AA network). However, the airport network doesn’t have any links at distances smaller than $10^2$ kilometers, while the maximal distance in this dataset is limited because we consider only connections within India. Consequently, the distance values of the airport network are concentrated on large distances without much spread. On the other hand, the train stations have a much wider spread as they include minor train stations as well. In that aspect, since the datasets are limited to India, the probability of an airport long distance connection always remains larger than the probability of a long distance railway connection.

5.6 Concluding Remarks

In this chapter, we introduced the statistical mechanics of multiplex and interacting spatial network ensembles. A large variety of multiplexes and interacting networks that are embedded in a real or hidden space can be characterized by this approach. We demonstrated analytically that spatial multiplexes, unlike uncorrelated sparse multiplexes, naturally develop a significant overlap of links. This shows that the empirical observations of significant overlap occurring in multiplex datasets, such as transportation multiplexes and social multiplexes, may be caused by their underlying geometry. We also built ensembles of interacting spatial networks and as a case study we investigated the interacting railway and airport networks of India. In the framework of randomized interacting spatial network ensembles, we measured the function $W(d)$ that modulates the link probability
Figure 5.4: Plot of $W(d)$ the factor that depends on the distance $d$ between the nodes and that affects the link probabilities, for the Indian railway network (RR), Indian airport network (AA) and the bipartite network of interconnections between airports and train stations (AR). At large distance the functions $W(d)$ for the three networks decay as a power-law of distance $W(d) \propto d^{-\delta}$, with the value of the fitted exponent $\delta$ indicated in the figure.
between two nodes at a distance \( d \) in the randomized airport (AA), railway (RR) and interconnection (AR) networks, showing that the function \( W(d) \) decays as a power-law of distance for large distances in all three cases.

As a prospective course of research, this analysis could be extended to directed and weighted networks. For example, the railway and air transportation networks could be generalized to accommodate the traditional weighted networks approach in transportation where the weight of each link is given by the number of trains (or flights) between two nodes. Furthermore, complex multiplex and interacting spatial networks are usually co-evolving and interdependent as demonstrated by the case of well-integrated transportation systems with an efficient transfer system from railway stations to airports and vice versa. Earlier studies have dealt with the onset of interdependence in Chinese and European railway-airline transportation networks [262]. However, it lacked the spatial aspect between the layers of interdependent networks. In the future, the analysis presented here can be expanded by developing a generalized framework to model and predict the efficient functioning of various multilayered spatial networks.
Chapter 6

Conclusion

Complex networks are dynamic objects by nature. They are subject to evolution by network growth, i.e. gradual expansion by the addition of new nodes, and are also defined by temporal characteristics due to links appearing and disappearing in time. Exploring their dynamics has thus been one of the main concerns of complex network research starting from the preferential attachment model. In this thesis, we have addressed the advantages and consequences of taking a dynamic approach to their description. As part of this approach, we have studied the entropy rate of various growing network models, which acts as a proxy of their complexity and information content, by calculating the typical number of networks generated by them and comparing it to the number of static networks with the same degree distribution created by the configuration model. We have shown how stochastic dynamic models such as the duplication-divergence model can be used to generate particular properties of complex networks such as monochromaticity, which constitute hard constraints if imposed on the links of a static network.

Another very important property of complex networks is that they are known to sustain many types of dynamical processes. These dynamical processes result in significantly different properties compared to regular topologies. The investigation of quantum dynamical processes is relatively new to complex network research. In this thesis, we have provided two instances of quantum critical phenomena defined on complex topologies. We have demonstrated that similar to classical critical phenomena, quantum dynamics is also affected by a complex topology. Moreover, dynamical processes are prone to be affected profoundly by a multilayered complex topology. In line with this up-and-coming field of research, we have studied two dynamical processes on multiplex and interacting networks.
We have shown with an election model how the dynamical exchange of opinions between two interacting layers reveals the importance of connectivity and committed voters. We have also shown how the dynamics of biased random walks on multiplex networks uncovers a centrality ranking that is different from the one defined on single layers. Finally, the dynamics of multilayered networks is likely affected by spatial properties, which we have explored by showing the emergence of significant link overlap and improved navigability on multiplex and interacting spatial networks.

The work presented in this thesis can be extended in many ways. The entropy rate serves as a further step towards an information theory of complex networks and can continue to be explored for many growing network models to quantify the information encoded in them. Even though modeling the evolution of monochromaticity as much as any other biological trait is a complicated task, our proposed epistatic growth models can be considered a first step in this direction and can inspire further efforts expanding their parameter space or doing a motif based search to supplement clinical studies. As far as research on the dynamics of multilayered networks goes, our election model captures the dynamics of a competition process on interacting networks and is motivating as an example of the many processes that can take place in a similar setting. As an extension to this study, the very same model can be applied to networks with different degree distributions (e.g. scale-free) to reflect different types of social ties. Considering the recent surge of interest in multiplex networks, the part on multiplex PageRank could well motivate further research on other multiplex centrality measures that take into account a node’s presence on other layers when assessing its importance in one layer. Since link overlap is widely encountered in real-world networks and is shown to be very influential in the dynamics of multilayered networks, we believe that our analytical demonstration of the onset of overlap might provide a plausible and mathematically sound explanation of this observation in real-life networks. Moreover, it provides a good example of the use of statistical mechanics on complex problems involving interacting transportation networks in an era when large scale multiplex datasets on space and mobility are increasingly becoming available.

To conclude, the complex interplay between the dynamics and structure of complex networks offer a very rich class of problems. In this dissertation, we addressed current challenges pertaining to the dynamics of and on complex networks by taking a multifaceted approach in tackling this broad subject, with a focus on a wide variety of networks including social, biological, transportation and quantum networks. We expect that in the future
the different spatio-temporal aspects of networks and multilayer topologies will be linked
to the behavior of their dynamics. In particular, correlations existing in these networks
will strongly affect their dynamics. On the quantum side, we expect that the interplay
between quantum dynamics and complex topologies will become ever more relevant in the
near future as experimental realizations of such quantum systems, in the context of ultra-
cold atom physics and quantum optics/quantum information, become more amenable to
complex architectures. As an example, the embedding of quantum systems in complex ar-
chitectures by long-range connections may ultimately pave the way for a quantum internet.
There is no question that the elucidation of the dynamical aspects of complex networks
will continue to be pursued on all fronts, especially in the multilayered/multiplex frame-
work, culminating in the discovery of new phenomena and more realistic models where
real-world network characteristics are captured in a more complete way. We believe that
the work embodied in this dissertation offers a useful contribution to this ongoing effort.
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Appendix

A.1 Mean field solution of the JCH model

The Jaynes-Cummings Hamiltonian (we set $\hbar = 1$)

$$H_{JC} = \epsilon \sigma^+ \sigma^- + \omega a^\dagger a + \beta (\sigma^+ a + \sigma^- a^\dagger) \quad (A.1)$$

is obtained in the rotating wave approximation and in the limit $\beta \ll \epsilon, \omega$. The total number of excitations is a conserved quantity, and it is given by the sum of electromagnetic and atomic excitations $N = a^\dagger a + \sigma^+ \sigma^-$. The interacting part of the Hamiltonian connects $n$-sectors which differs only by one photon excitation

$$|n - 1\rangle |\uparrow \rangle \leftrightarrow |n\rangle |\downarrow \rangle \quad (A.2)$$

The JC Hamiltonian can then be block-diagonalized in different sectors, each labelled by $n$, and each sector spanned by $\{|n - 1\rangle |\uparrow \rangle, |n\rangle |\downarrow \rangle\}$. Choosing this set as the basis for the $n$–th sector, Eq.(3.23) and Eq.(3.25) in the main text provide the expressions for the eigenvectors and eigenvalues of the JC Hamiltonian.

Considering the situation of a network of cavities, whose coupling is effectively described by an hopping term, we have the Jaynes-Cummings-Hubbard Hamiltonian described in Eq.(3.27). As explained in the main text, the mean-field treatment of the
hopping term allows us to approximate the JCH Hamiltonian as follows

\[ H^{MF} = \sum_i \epsilon \sigma_i^+ \sigma_i^- + \omega a_i^+ a_i + \beta (\sigma_i^+ a_i + \sigma_i^- a_i^+) \]
\[ -\kappa \sum_{i,j} \tau_{ij} (a_i^+ + a_i) \psi_j + \kappa \sum_{i,j} \tau_{ij} \psi_i \psi_j. \]

Considering the hopping term as a perturbation to the atomic limit, the order parameter of the model is provided by \[ \psi_i \equiv \langle a_i \rangle_{gs} \], where the expectation value is calculated with respect to the ground-state of the Jaynes-Cummings-Hubbard model to first order in perturbation theory. Note that the order parameter can be assumed real due to the gauge symmetries of the Hamiltonian [159]. The self-consistent equation for the order parameter can then be written as

\[ \psi_i \equiv \langle n_1 | a_i | n_1 \rangle, \quad (A.3) \]

where \(|n_1\rangle \equiv |n, -\rangle^0 + |n\rangle^1\) is the approximation of the ground-state to first-order in the perturbation, while \(|n, -\rangle^0\) is the ground-state of the unperturbed Hamiltonian (see Eq.3.23 in the main text), and

\[ |n\rangle^1 = \sum_{k,\alpha=\pm} 0 \langle k, \alpha | H^{MF}_{hop} | n, -\rangle^0 \frac{E_{n,-}^\mu}{E_{n,-}^\mu - E_{k,\alpha}^\mu} | k, \alpha \rangle^0. \]

From Eq. (A.3) we have

\[ \langle n_1 | a_i | n_1 \rangle = 0 \langle n, - | a_i | n, - \rangle^0 + 1 \langle n | a_i | n \rangle^1 \]
\[ + 0 \langle n, - | a_i | n \rangle^1 + 1 \langle n | a_i | n, - \rangle^0. \]

Keeping only non-zero terms to first order in \(\kappa\) we are left only with the last two terms in the above equation. First we explicitly calculate

\[ 0 \langle n, - | a_i | n \rangle^1 = \sum_{k,\alpha=\pm} 0 \langle k, \alpha | H^{MF}_{hop} | n, -\rangle^0 \frac{E_{n,-}^\mu}{E_{n,-}^\mu - E_{k,\alpha}^\mu} 0 \langle n, - | a_i | k, \alpha \rangle^0. \]

It is easy to check that the only non-zero terms in the sum are given by \(k = (n + 1), \alpha = +, -\). It follows that the non-zero contribution to the expectation value of \(H^{MF}_{hop}\) is provided only by \(-\kappa \sum_j \tau_{ij} a_i^+ \psi_j\). From the explicit form for the ground-states of the
unperturbed Hamiltonian (see Eq.3.23 in the main text) we obtain

\[ 0\langle n, -|a_i|(n + 1), -\rangle^0 = \sqrt{n + 1} \cos \theta_n \cos \theta_{n+1} + \sqrt{n} \sin \theta_n \sin \theta_{n+1} \]

\[ 0\langle n, -|a_i|(n + 1), +\rangle^0 = \sqrt{n + 1} \cos \theta_n \sin \theta_{n+1} - \sqrt{n} \sin \theta_n \cos \theta_{n+1}. \]

We can proceed similarly for the calculation of \( 1\langle n|a_i|n, -\rangle^0 \), obtaining

\[ 0\langle (n - 1), -|a_i|n, -\rangle^0 = \sqrt{n} \cos \theta_n \cos \theta_{n-1} + \sqrt{n - 1} \sin \theta_n \sin \theta_{n-1} \]

\[ 0\langle (n - 1), +|a_i|n, -\rangle^0 = \sqrt{n} \cos \theta_n \sin \theta_{n-1} - \sqrt{n - 1} \sin \theta_n \cos \theta_{n-1}. \]

Now let us define

\[ R_n \equiv -\sum_{\alpha=\pm} \frac{|\langle n, -|a_i|(n + 1), \alpha\rangle^0|^2}{E_{n,-}^\mu - E_{(n+1),\alpha}^\mu} + \frac{|\langle (n - 1), \alpha|a_i|n, -\rangle^0|^2}{E_{n,-}^\mu - E_{n-1,\alpha}^\mu}. \]

Putting everything together we have the following self-consistent equation to first order in perturbation theory (for \( n > 0 \))

\[ \psi_i = \kappa R_n \sum_j \tau_{ij} \psi_j, \]

The case \( n = 0 \) can be calculated in the same way and one has

\[ \psi_i = \kappa R_0 \sum_j \tau_{ij} \psi_j, \]

where

\[ R_0 = -\sum_{\alpha=\pm} \frac{|\langle 0, \downarrow|a_i|1, \alpha\rangle|^2}{E_{0,\downarrow}^\mu - E_{1,\alpha}^\mu}, \]

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with \( \langle 0, \downarrow | a_i | 1, - \rangle = \cos \theta_1 \), and \( \langle 0, \downarrow | a_i | 1, + \rangle = \sin \theta_1 \).

### A.2 Approximating Multiplex PageRank by the degree.

In order to calculate the Multiplex PageRank \( X_i \) of node \( i \), we use an iterative procedure. PageRank \( X^n = \{ X^n_1, \ldots, X^n_N \} \) at time step \( n \) can then be calculated from PageRank \( X^{n-1} \) at time step \( n - 1 \) according to the recursive equation

\[
X^n_i = \alpha_B \sum_j x_i^B B_{ij} \frac{X^{n-1}_j}{G_j} + (1 - \alpha_B) \frac{x_i^\gamma}{\langle x^\gamma \rangle_N},
\]

(A.4)

where PageRank \( X_i \) is given by \( X_i = \lim_{n \to \infty} X^n_i \) and where \( G_j = \sum_r B_{rj} x_r^B + \delta(0, \sum_r B_{rj} x_r^B) \).

Following [234, 235], we divide the PageRank of nodes in network B into different classes, where two or more nodes belong to the same class if they have the same in- and out-degree and the same PageRank \( x \). We define \( \overline{X}(k^{(B)}, x) \) as the average value of the PageRank of nodes in the degree class \( k^{(B)} = (k_{in}^{(B)}, k_{out}^{(B)}) \) in network B and with PageRank \( x \) in network A

\[
\overline{X}(k^{(B)}, x) = \frac{1}{NP(k^{(B)}, x)} \sum_{i|k_i^{(B)}=k^{(B)}, x_i=x} X_i,
\]

(A.5)

where \( P(k^{(B)}, x) \) is the probability that a node has degree \( k^{(B)} \) in network B and PageRank \( x \) in network A. Similarly, we define \( \overline{X'}(k^{(B)}, x) \) from the iterative procedure

\[
\overline{X'}^n(k^{(B)}, x) = \frac{1}{NP(k^{(B)}, x)} \sum_{i|k_i^{(B)}=k^{(B)}, x_i=x} X_i^n
\]

\[
= \frac{\alpha_B}{NP(k^{(B)}, x)} \left( \sum_{i|k_i^{(B)}=k^{(B)}, x_i=x} \sum_j x_i^B B_{ij} \frac{X^{n-1}_j}{G_j} \right) + (1 - \alpha_B) \frac{x_i^\gamma}{\langle x^\gamma \rangle_N},
\]

(A.6)

The term \( G_j \) in the above equation can be approximated as

\[
G_j = \sum_r x_r^B B_{rj} + \delta(0, k_{j, out}^{(B)}) \simeq k_{out, j}^{(B)} \sum_{k^{(B)}, x_j} P_{out}^{(B)}(k^{(B)}, x_j | k_j^{(B)}, x_j) x_j^B + \delta(0, k_{j, out}^{(B)}),
\]

(A.7)

where \( P_{out}^{(B)}(k^{(B)}, x_j | k_j^{(B)}, x_j) \) is the probability of reaching a node with degree \( k^{(B)} \) and PageRank \( x' \) by following a link in network B from a node of degree \( k_j^{(B)} \) and PageRank \( x_j \). If the nodes belonging to class \( \{ k_j^{(B)}, x_j \} \) are uncorrelated to the nodes of class \( \{ k^{(B)}, x \} \),
then

\[ P^{(B)}_{\text{out}}(k'_{j}, x'|k_j^{(B)}, x_j) = \frac{k_{\text{in}}^{(B)}}{\langle k_{\text{in}}^{(B)} \rangle} P(k^{(B)}, x' ) , \quad (A.8) \]

such that

\[ G_j \simeq k_{\text{out}, j}^{(B)} \frac{\langle x^{\beta} k_{\text{in}}^{(B)} \rangle}{\langle k_{\text{in}}^{(B)} \rangle} + \delta(0, k_{\text{out}}^{(B)}). \quad (A.9) \]

Using the approximation for \( G_j \) we can express the sum in Eq. (A.6) via a mean–field approximation, obtaining

\[
\sum_{i[k]^{(B)}=k^{(B)}, x_i=x} \ x_i B_{ij} \frac{X_{j}^{n-1}}{G_j} = \sum_{k''} \sum_{x''} \sum_{i[k]^{(B)}=k^{(B)}, x_i=x} x_i B_{ij} \frac{X_{j}^{n-1}}{\langle k_{\text{in}}^{(B)} \rangle} \frac{\langle k_{\text{in}}^{(B)} \rangle}{\langle x^{\beta} k_{\text{in}}^{(B)} \rangle} \delta_{ij} \sum_{j[k]^{(B)}=k''} B_{ij} \approx \sum_{k''} \sum_{x''} \sum_{i[k]^{(B)}=k^{(B)}, x_i=x} X_{j}^{n-1} \frac{\langle k_{\text{in}}^{(B)} \rangle}{\langle x^{\beta} k_{\text{in}}^{(B)} \rangle} \frac{\langle k_{\text{in}}^{(B)} \rangle}{\langle k_{\text{out}}^{(B)} \rangle} \delta_{ij} \sum_{j[k]^{(B)}=k''} B_{ij} \sum_{j[k]^{(B)}=k''} B_{ij} \quad \text{(A.10)}
\]

where we used the mean–field approximation

\[ \sum_{j[k_j^{(B)}=k''}] X_{j}^{n-1} B_{ij} \simeq X_{j}^{n-1}(k^{(B)}, x'') \sum_{j[k_j^{(B)}=k''}] B_{ij} \quad \text{(A.10)} \]

and \( P^{(B)}_{\text{in}}(k''(B), x''|k^{(B)}, x) \) is the probability that, by following an incoming link of a node with degree \( k^{(B)} \) and PageRank \( x \) in network B, a predecessor of the node with degree \( k''(B) \) and PageRank \( x'' \) can be reached. In an uncorrelated network, this quantity is given by

\[ P^{(B)}_{\text{in}}(k''(B), x''|k^{(B)}, x) = \frac{k_{\text{out}}^{(B)}}{\langle k_{\text{in}}^{(B)} \rangle} P^{(B)}(k''(B), x''). \quad (A.11) \]

Inserting Eqs. (A.10) and (A.11) in Eq. (A.6), and taking the limit \( n \to \infty \), we obtain

\[ \overline{X}(k^{(B)}, x) = \alpha_B \frac{x^{\beta} k_{\text{in}}^{(B)}}{\langle x^{\beta} k_{\text{in}}^{(B)} \rangle N} + (1 - \alpha_B) \frac{x^{\gamma}}{N \langle x^{\gamma} \rangle}, \quad (A.12) \]
where the values of $x$ can be approximated from Eq. (4.4)

$$\overline{x}(k^{(A)}) = \alpha_A \frac{k_{in}^{(A)}}{\langle k_{in}^{(A)} \rangle_N} + (1 - \alpha_A) \frac{1}{N}. \quad (A.13)$$

### A.3 Extension of Multiplex PageRank to multiplex networks with more than two layers.

The proposed Multiplex PageRank centrality measure, presented in the main text for the specific case of a duplex network, can easily be extended to multiplex networks with more than two layers. Let us consider a multiplex network with $M$ layers given in a predetermined order, where each layer $\ell = 1, 2, \ldots, M$ corresponds to a network with adjacency matrix $A^{(\ell)}_{ij}$. We can define the Multiplex PageRank $X^{(\ell)}_i$ recursively in the following way. At the first level of the iteration $\ell = 1$, we have the single-layer PageRank $X^{(1)}_i$ defined as

$$X^{(1)}_i = \alpha^{(1)} \sum_j A^{(1)}_{ij} \frac{X^{(1)}_j}{G^{(1)}_j} + (1 - \alpha^{(1)}) \frac{1}{N}, \quad (A.14)$$

where $G^{(1)}_j = \max(1, \sum_r A_{rj})$. We then include the information about the structure of the other layers, and obtain

$$X^{(\ell)}_i = \alpha^{(\ell)} \sum_j \left[ X^{(\ell-1)}_i \right]^\beta A^{(\ell)}_{ij} \frac{X^{(\ell)}_j}{G^{(\ell)}_j} + (1 - \alpha^{(\ell)}) \frac{\left[ X^{(\ell-1)}_i \right]^\gamma}{N \left\langle \left[ X^{(\ell-1)} \right]^\gamma \right\rangle}, \quad (A.15)$$

where $G^{(\ell)}_j = \sum_r A^{(\ell)}_{rj} \left[ X^{(\ell-1)}_r \right]^\beta + \delta \left( 0, \sum_r A^{(\ell)}_{rj} \left[ X^{(\ell-1)}_r \right]^\beta \right)$. For the sake of simplicity, here we have chosen exponents $\beta$ and $\gamma$ that do not depend on $\ell$, but in general it is also possible to consider the case in which the exponents $\beta$ and $\gamma$ are dependent on the layers $\ell$. 
A.4 Expected overlap in multiplex ensembles with link probability decaying like a power-law with distance

In order to generalize the results proven in paragraph 5.4.2.1, we evaluate here the expected overlap for a multiplex ensemble with link probability decaying as a power-law of the distance. In particular the link probability in the generic layer $\alpha$ satisfies Eq. (5.43), where each $P_\alpha(G_\alpha|\{r_i\})$ is given by Eq. (5.44) and where $p_{\alpha ij}(d_{ij})$ is given by Eq. (5.22), i.e.

$$p_{\alpha ij}(d_{ij}) = \frac{\theta_i^\alpha \theta_j^\alpha r^{-\delta_\alpha}}{1 + \theta_i^\alpha \theta_j^\alpha r^{-\delta_\alpha}}. \quad (A.16)$$

The “hidden variables” $\theta_i^\alpha$ fix the expected degree of node $i$ in layer $\alpha$, i.e.

$$\kappa_i^\alpha = \sum_j p_{\alpha ij}(d_{ij}), \quad (A.17)$$

and the “hidden variables” $\delta_\alpha$ fix the total cost $L^\alpha = N\ell^\alpha$ given by Eq. (5.18) associated with the links in layer $\alpha$ that we rewrite here for convenience

$$L^\alpha = N\ell^\alpha = \sum_{i<j} \log(d_{ij}) p_{\alpha ij}(d_{ij}). \quad (A.18)$$

Let us consider for simplicity the case in which all the expected degrees in the same layer are equal and finite, i.e. $\kappa_i^\alpha = \kappa^\alpha \forall i$. Moreover let us make the additional assumption that the nodes are distributed uniformly in a $D$ dimensional Euclidean hypersphere of radius $R$, with density $\rho$. In this hypothesis, following a procedure similar to the one presented in detail in paragraph 5.4.2.1, we get that the relation between $(\kappa^\alpha, L^\alpha = N\ell^\alpha)$ and the “hidden variables” $(\theta^\alpha, \delta_\alpha)$ is given, in the continuous approximation and in the limit $R, N \to \infty$ by

$$\kappa^\alpha = \rho \Omega(D) \sum_{n=0}^\infty (\theta^\alpha)^{2(1+n)} \frac{(-1)^n}{\delta_\alpha(1+n) - D} \quad (A.19)$$

$$\ell^\alpha = \rho \frac{\Omega(D)}{2} \sum_{n=0}^\infty (\theta^\alpha)^{2(1+n)} \frac{(-1)^n}{[\delta_\alpha(1+n) - D]^2} \quad (A.20)$$

as long as $\delta_\alpha > D$. Therefore, the ”hidden variables” $(\theta^\alpha, \delta_\alpha)$ are finite. The expected total and local overlap between layer $\alpha$ and layer $\alpha'$ are given by Eqs.(5.37) that we can
estimate in the continuous approximation and in the thermodynamic limit \( R, N \to \infty \).

We have in particular

\[
\left\langle O^{\alpha,\alpha'} \right\rangle = N \frac{1}{2} \rho \Omega(D) J(\alpha, \alpha')
\]

\[
\left\langle o^{\alpha,\alpha'} \right\rangle = \rho \Omega(D) J(\alpha, \alpha') \tag{A.21}
\]

where \( J(\alpha, \alpha') \) is finite and given by

\[
J(\alpha, \alpha') = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \theta^\alpha \right)^{2(n+1)} \left( \theta^{\alpha'} \right)^{2(m+1)} \times \\
\times \frac{1}{\delta^\alpha (1 + n) + \delta^{\alpha'} (1 + m) - D}. \tag{A.22}
\]

Given the Eqs. (A.21) we can conclude that also in this case a finite fraction of links are overlapping between any two layers and that this overlap is distributed uniformly over the network.

A.5 Expected overlap in multiplexes with some layers having a link probability decaying exponentially with distance and other layers having a link probability decaying as a power-law

Here we evaluate the expected overlap in multiplex ensembles with some networks with link probability decaying exponentially with distance and with the other networks with link probability decaying as a power-law of the distance between the linked nodes. In particular the different layers will have a link probability satisfying Eq. (5.43), where the probabilities \( P_\alpha(G_\alpha|\{\vec{r}_i\}) \) are given by Eq. (5.44) where \( p_i^\alpha(d_{ij}) \) for some layers is given by Eq. (5.21), for other layers is given Eq. (5.22). In other words the link probability in some layers is decaying exponentially with distance and in some other layers is decaying as a power-law of the distance. The “hidden variables” \( \theta^\alpha_i \) fix the expected degree of node \( i \) in layer \( \alpha \), i.e.

\[
\kappa^\alpha_i = \sum_j p^\alpha_{ij}(d_{ij}), \tag{A.23}
\]
and the “hidden variables” δ_α or d_α fix the total cost L^α = Nℓ^α associated with the links in layer α given by

\[ L^\alpha = N\ell^\alpha = \sum_{i<j} f_\alpha(d_{ij})p_{ij}^\alpha(d_{ij}). \] (A.24)

where \( f_\alpha(d_{ij}) = \log(d_{ij}) \) or \( f_\alpha = d_{ij} \) depending on the layer α. Let us consider for simplicity the case in which all the expected degrees in the same layer are equal and finite, i.e. \( \kappa_i^\alpha = \kappa^\alpha \) \( \forall i \). Moreover let us make the additional assumption that the nodes are distributed uniformly in a Euclidean D dimensional hypersphere of radius \( R \), with density \( \rho \). For each network in each layer the “hidden variables” (\( \theta^\alpha, d_\alpha \)) can be found using the Eqs. (5.50) – (5.51), while the “hidden variables” (\( \theta^\alpha, \delta_\alpha \)) can be found using the Eqs. (A.19), (A.20). If we consider two layers with link probability decaying exponentially with distance we have that their expected global and local overlap is given by Eqs (5.53) – (5.55), if we have two layers with link probability decaying as a power-law we find instead Eqs. (A.21), (A.22). Finally if we have two layers, a layer α with link probability decaying exponentially with distance, and a layer α’ with link probability decaying as a power-law of the distance between the nodes, the expected total and global overlap between these two layers is given by

\[ \langle O^{\alpha,\alpha'} \rangle = N\rho\Omega(D)K(\alpha,\alpha') \]
\[ \langle o^{\alpha,\alpha'} \rangle = \rho\Omega(D)K(\alpha,\alpha') \] (A.25)

where \( K(\alpha,\alpha') \) is finite and given by

\[ K(\alpha,\alpha') = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (\theta^\alpha)^{2(n+1)} (\theta^\alpha')^{2(m+1)} \times \]
\[ \times E_{1+\delta_{\alpha'}(1+m)-D}(\frac{1}{d_\alpha}), \] (A.26)

where \( E_n(z) \) is the exponential integral function. Therefore, also in the case in which a spatial multiplex is formed by some networks with link probability decaying exponentially with the distance and other networks with link probability decaying as a power-law of the distance, the expected global and local overlap is significant.